Integration of Second Generation Biofuel Production into Existing Industrial Processes for Short Term Commercial Implementation

by

Abdul Muhaymin Petersen

Dissertation presented for the Degree

of

DOCTOR OF PHILOSOPHY
(Chemical Engineering)

in the Faculty of Engineering
at Stellenbosch University

Supervisor
Professor Johann Gorgens

December 2015

Declaration

By submitting this dissertation electronically, I declare that the entirety of the work contained therein is my own, original work, that I am the sole author thereof (save to the extent explicitly otherwise stated), that reproduction and publication thereof by Stellenbosch University will not infringe any third party rights and that I have not previously in its entirety or in part submitted it for obtaining any qualification.

This dissertation includes 3 original papers published in peer reviewed journals. The development and writing of the papers (published and unpublished) were the principal responsibility of myself and, for each of the cases where this is not the case, a declaration is included in the dissertation indicating the nature and extent of the contributions of co-authors.

Date: 04-November-2015

Abstract

Since the production of second-generation biofuel (SGB) from lignocellulosic plant biomass is only economically attractive if driven by government incentives, stakeholders are reluctant to commercialise the product despite its potential to mitigate global warming and socio-economic conditions. Integrating SGB processes with the facilities of biomass-based industries could reduce the production costs of SGB through pre-existing services and infrastructure. Integrating SGB, however, is technically viable only if available biomass residues are used effectively to co-produce fuel while maintaining the overall energy balance, financially viable only if it attracts private investment without governmental assistance and environmentally viable only if it reduces the carbon imprint of a fossil-intensive host industry.

In this dissertation, novel scenarios for integrating SGB with the South African raw sugar and the pulp and paper industries (RSI and P&PI, respectively) were explored. Focus was on ethanol production based on fermenting hemicellulose substrates, potentially available in both industries, and on SGB production through gasification-synthesis processes in the contextual representatives of these industries. This was accomplished through flow-sheet analysis in Aspen Plus® using process simulations constructed from protocols in published literature and experimental data.

In respect of RSI, integrating bioethanol production with electricity from sugarcane bagasse and harvesting residues were deemed both technically and economically viable and competitive against the exclusive generation of electricity. The necessity of Pinch Point Analysis was established through flow-sheet analysis, which had also shown the synergistic interaction of technologies in various processing stages, such as the variants in ethanol distillation technologies and heat and power production technologies. In respect of P&PI, represented by sulphite mills, ethanol production from spent sulphite liquor (SSL) pulping residue was deemed economically viable if the SSL fermentation

substrate was concentrated. To attain net reduction of greenhouse gas emissions for the integrated ethanol-sulphite facility, it was essential to provide all process energy requirements from supplementary biomass sources rather than coal.

In respect of RSI, integrating methanol or Fischer-Tropsch syncrude via gasification synthesis was deemed not feasible at the current state of efficiency with which sugar mills are operating. In respect of P&PI, combining synthetic fuel production with bioethanol production at a sulphite mill improved economic potential, since disposal costs were negated through the use of waste biomass for synthesis processes and the yield of valuable products was enhanced on a small scale. In respect of both RSI and P&PI, however, integrating gasification-synthesis processes required the statistical optimisations of flow sheets to arrive at the optimum operating parameters for competing technologies for syngas production. In these contexts, syngas production based on optimised allothermal gasification had lower costs than optimised autothermal gasification.

To validate the process concepts developed in this thesis, it is firstly recommended that robust and recombinant microbial strains be readily available to ferment pentose-rich substrates, such as SSL and hemicellulose hydrolysates. Secondly, the effect of the chemical alteration of SSL on the recovery performance of process chemicals at sulphite mills should be examined and, thirdly, the catalytic gasification of biomass should be developed and demonstrated on pilot and pre-commercial scales.

Opsomming

Aangesien die produksie van tweedegenerasie-biobrandstof (TGB) uit lignosellulosiese plantbiomassa slegs ekonomies aantreklik is indien dit deur staatsaansporings aangemoedig word, is belanghebbendes huiwerig om die produk te kommersialiseer, ondanks die potensiaal daarvan om aardverwarming teen te werk en sosio-ekonomiese omstandighede te verbeter. Die integrasie van TGB-prosesse by die fasiliteite van biomassagebaseerde nywerhede kan die produksiekoste van TGB verlaag deur voorafbestaande dienste en infrastruktuur. Die integrasie van TGB is egter slegs tegnies haalbaar indien die beskikbare biomassareste doeltreffend gebruik word vir die medeproduksie van brandstof terwyl die algehele energiebalans terselfdertyd gehandhaaf word; slegs finansieel haalbaar indien dit privaat belegging sonder staatshulp lok, en slegs omgewingshaalbaar indien dit die koolstofvoetspoor van ’n fossielintensiewe gasheernywerheid verklein.

Hierdie verhandeling verken nuwe scenario’s vir die integrasie van TGB by die Suid-Afrikaanse ru-suiker- en pulp-en-papierbedryf (RSB en P&PB onderskeidelik). Die klem val op etanolproduksie op grond van die fermentasie van hemisellulose-substrate, wat moontlik in albei nywerhede beskikbaar is, en op TGB-produksie deur vergassingsinteseprosesse in die kontekstuele verteenwoordigers van die twee nywerhede. Dít is gedoen met behulp van vloeikaartontleding in Aspen Plus®, wat gebruik gemaak het van prosessimulasies wat op grond van protokolle in gepubliseerde literatuur en eksperimentele data saamgestel is.

Wat RSB betref, blyk die integrasie van bio-etanolproduksie en elektrisiteit uit suikerrietbagasse en oesreste tegnies én ekonomies haalbaar te wees, sowel as mededingend vergeleke met die uitsluitlike opwekking van elektrisiteit. Die vloeikaartontleding het ’n behoefte aan knyppuntanalise uitgewys, wat ook gedui het op die sinergistiese wisselwerking tussen tegnologieë in verskillende verwerkingstadia, soos verskillende etanolsuiwering en hitte- en kragproduksie tegnologieë. Met

betrekking tot P&PB, in soverre dit deur sulfietmeule in Suid-Afrika verteenwoordig word, word etanolproduksie uit gebruikte sulfietloog (GSL), synde ’n pulp-residu, as ekonomies haalbaar beskou indien die GSL-fermentasiesubstraat gekonsentreerd is. Om ’n netto vermindering in kweekhuisgasvrystellings vir die geïntegreerde etanolsulfietfasiliteit te verkry, moet daar met behulp van aanvullende biomassabronne eerder as steenkool in alle prosesenergievereistes voorsien word.

By RSB blyk die integrasie van metanol of Fischer-Tropsch- sintetiese ruolie (“syncrude”) via vergassingsintese nie teen die huidige bedryfsdoeltreffendheid van die suikermeule uitvoerbaar te wees nie. Vir P&PB toon die kombinasie van sintetiese brandstofproduksie en bio-etanolproduksie by ’n sulfietmeul ekonomiese potensiaal, aangesien wegdoeningskoste geneutraliseer word deur die gebruik van afvalbiomassa vir sinteseprosesse en die kleinskaalse verhoging in die lewering van waardevolle produkte. Tog vereis die integrasie van vergassingsinteseprosesse by RSB sowel as P&PB die statistiese optimalisering van vloeikaarte om die optimale bedryfsparameters van wedywerende tegnologieë vir singasproduksie te bepaal. In hierdie verband blyk singasproduksie met behulp van geoptimaliseerde allotermiese vergassing meer kostedoeltreffend as geoptimaliseerde outotermiese vergassing te wees.

Vir die bekragtiging van die proseskonsepte wat uit hierdie tesis spruit, word daar eerstens aanbeveel dat robuuste en rekombinante mikrobiese stamme geredelik beskikbaar moet wees om pentoseryke substrate, byvoorbeeld GSL en hemisellulose-hidrolisate, te fermenteer. Tweedens behoort die uitwerking van die chemiese wysiging van GSL op die herwinningsprestasie van proseschemikalieë by sulfietmeule ondersoek te word. Laastens word aanbeveel dat die katalitiese vergassing van biomassa op ’n proef- sowel as prekommersiële skaal ontwikkel en gedemonstreer word.

Declarations of Contributions to the Work

Name of Co-author	e-mail Address	Nature of Contribution	Extent to the contribution by respective co-author
Mathew Aneke	mathew.aneke@gmail.com	Internal reviser, language editing, involved in Chapter 4.	30%
Kate Haigh	khaigh@sun.ac.za	Internal reviewer, language editing, involved in Chapter 5.	40%
Somayeh Farzad	somayeh_farzad1980@yahoo.com	- Gave research guidance on the technical content of Chapter 6 - Internal reviewer of Chapter 6 - Structure and presentation of Chapter 6.	60% 40% 50%
Johann Gorgens	jgorgens@sun.ac.za	- Sole internal reviewer of chapter 1,2,3,7 and 8. - Internal reviewer on grammar and language in Chapter 4, 5, 6, - Sole guide on technical aspects in Chapters 1, 2, 3, 4, 5, 7, 8. - Gave guidance in part in chapter 6.	100% 70% (Chapter 4) 60% (Chapter 5 &6) 100% 40%

Acknowledgements

I firstly acknowledge my Creator and Sustainer for giving me the strength and faculties to have undertaken this study.

I acknowledge my parents and family for their unconditional support.

I acknowledge my supervisor, Professor Johann Gorgens for his guidance throughout the duration of the project.

I acknowledge the National Research Foundation of South Africa for providing me with the bursary to undertake the project.

Table of Contents

List of Figures

List of Tables

Glossary of General Terms

Contextual	
Sugarcane Crushing Industry	Broad term applying to industries that processes sugarcane into products.
Raw Sugar Industry	An industry producing raw sugar from sugarcane.
Autonomous ethanol distilleries	An industry producing anhydrous ethanol from sugarcane.
Paper and Pulp Industry	An industry that processes woody biomass into chemical pulps or paper. The two variations are the Kraft and Sulphite Processes.
Biological process	A biofuel production process that has the fermentation of sugars to ethanol as the primary conversion process.
Gasification-synthesis process	A biofuels production process involving the conversion of biomass to syngas, which is in turn converted to synthetic fuels.
Technical and Environmental	
Feedstock	The starting material of the biofuel production process that ranges from crops, to plant matter and residues and then to industrial wastes.
Process simulation	Simulating the mass and energy balance of an industrial scale process in a computing environment in order to predict the performance of the process.
Heat Integration	Integrating the heat requirements and wastes of a process in order to improve the efficiency of a process.
Co-production	Producing a biofuel product, together with an electrical product, as saleable products.
Exclusive Electricity Generation	Converting feedstock in order to generate electricity as the only saleable product.
Exporting Efficiency / Net Energy Efficiency	The efficiency with an annexed or integrated bio-energy facility (such as biofuel or electricity production) can convert the total energy availability in the residues to a saleable energy product.
Fossil Fuel Displacement	When an existing industrial process that currently uses fossil based energy to fulfil its energy demands, then the *Fossil Fuel Displacement* measures the extent to which fossil energy is reduced through the integration of a bio-energy process.
Net Greenhouse Gas Reduction	The reduction in the amount of greenhouse gases that would the atmosphere, due to the existence of the biofuel production project under consideration.
Global Warming Potential	The product of the Net Greenhouse Gas Reduction and negative one (-1). It describes the extent to which a product life cycle contributes to global warming.
Economic	
Incentive	Where government provides an economic support for a biofuels project to justify an investment from stakeholders. It could be capital grants, or industrial development fund, tax rebates, depreciation

	allowances or subsidising the price paid to the biofuel producer per litre of fuel sold.
Commercial Investment	Loan provided by a commercial bank.
Private Investment	Investment from entities that are not affiliated to government or commercial banks.
Internal Rate of Return	The virtual interest gained on an investment in a business, and it is used to compare economic performance of a business against interest rates.
Financial Risk Assessment	Quantifying the probability of attaining a desired economic result.
Production Cost	The total cost involved in producing fuel, which involves the capital repayment and operational costs in producing a litre of fuel.

Abbreviations

Abbreviation	Description
SCCI	Sugarcane Crushing Industry
P&PI	Paper and Pulp Industry
RSI	Raw Sugar Industry
SSL	Spent Sulphite Liquor
TDS	Total dissolved solids
DAH	Dilute acid hydrolysis
STEX	Steam Explosion
CON/CD	Conventional Distillation
VD/ME	Vacuum distillation/ Multi-effect distillation
EE	Exclusive Electricity generation
CHPSC	Combustion with High Pressure Steam Cycle
BIGCC	Biomass Integrated Gasification and Combined Cycles
CFB	Circulating Fluidised Bed
HRSG	Heat Recovery Steam Generator
BTS	Biomass-to-energy (electricity and heat)
BG	Biodigestion
MTS	Methanol Synthesis
FT	Fischer-Tropsch
AUT-G	autothermal gasification
ALO-G	allothermal gasification
AME	Amortised Capital Expenditure
CSP	Cost of Syngas Production

OOC	operational opportunity cost
CE	Conversion Efficiency
KEI	Key Economic Indicator
TCI	Total Capital Investment
Prob(X)	Probability of X
IRR	Internal Rate of Return
MESP/MFSP	Minimum Ethanol/Fuel Selling Price
GWP	Global Warming Potential
NGGRP	Net Greenhouse Gas Reduction Potential

Chapter 1: Introduction

1 Background to Investigation

The need for biofuels as an energy source for transportation has become imperative from a number of perspectives. Firstly, they serve as a means of providing energy security by substituting the use of fossil based fuels by those based on renewable sources[1,2]. Secondly, they provide a means of reducing the effects of global warming by reducing the output of greenhouse gases into the atmosphere associated with fossil fuel use[3,4]. Thirdly, they provide a means of stimulating the economies of developing countries through rural development[5], and thereby also improve national energy security. The production of biofuels from agricultural waste, for example, adds value to the waste products for rural farmers, hence providing a revenue if sold to a biofuel producer. Thus, given this crucial set motivating impetus, the South African government legislated in 2007 that biofuels would represent at least 2% of the usage of transportation fuels in South Africa by 2013[6,7]. This target however, has not been met, partly due to limited incentives that have not created sufficient returns on investment, to attract private capital into the renewable fuel sector in South Africa.

The production of biofuels by first generation technologies, though well understood and profitable when supported by financial incentives, is tightly regulated. This is primarily due to its inherent challenges it poses to the food industry, because such processes rely on raw materials that readily produces fermentable sugars, and has frequently utilised food crops for this purpose[8,9]. If first generation biofuel production is left unregulated, it could cause a shortage in food for human consumption [10] and potentially lead to water shortages due to consumption and contamination of water resources during the life cycle of the biofuel. Second generation of biofuel production bypasses several of the limitations of first generation technologies, by utilising non-food,

lignocellulosic (fibrous) plant biomass or industrial wastes as feedstock[11,12], which are in greater abundance than food-crops. The first examples of commercial scale production of second generation biofuels from lignocellulose are presently under development. The primary reason for the slow uptake of second generation biofuel technologies into the commercial space seems to be the uncertainty around the economic feasibility[11]. Indeed, most studies have indicated that second generation biofuel based on current technology is economically unfeasible. Financial viability may come in time along the learning curve of the technology development, so governmental assistance would be currently needed to achieve full financial viability later. Second generation biofuels are typically more expensive to produce than first generation biofuels, and further technology improvement is often proposed as a means to reduce the intensive capital and operational costs[13–15], while improving efficiency to afford an economic attraction[16]. Costs of second generation feedstock, even though much less than the cost of first generation feedstock, also constitutes a significant portion of operational costs of second generation fuels and thus a reasons for the poor financial prospects of second generation fuel[17,18].

Two competing forms of second generation biofuels obtained from lignocellulose are cellulosic ethanol (Bioethanol) and synthetic fuels (bio-synfuels). Bioethanol is produced from biomass through pre-treatment, biological conversion (hydrolysis-fermentation) and purification (i.e. biological route), while bio-synfuels are produced by gasification, Fischer-Tropsch synthesis and refining[19,20]. Bioethanol production is typically characterised by high production costs due to its thermal energy needed in pre-treatment and distillation, and its requirement for speciality reagents such as the enzymes needed for cellulose hydrolysis[13,21,22]. Bio-synthetic fuel production on the other hand is energy self-sufficient and does not carry significant process costs, but the high capital investment and feedstock costs required have usually been the reason that acceptable returns were not possible[15]. Thus, in most cases, second generation biofuel, produced by either the biological or gasification-synthesis routes, can only be implemented with significant financial incentives from

government, such as capital grants, subsidies and mandated price premiums for the biofuel product. As it had been shown that first generation processes have better financial feasibility than second generation processes, it can be expected that the incentives required for second generation will be higher[14]. It is often argued that this initial governmental aid for commercialising second generation biofuel production at the current pioneer level would enable a technological learning curve that with time will eventually decrease production costs, such that n^{th} technological costs can be achieved[21].

Therefore, the short-term commercial implementation of second generation biofuel production requires solutions that bypass the financial hurdles imposed by the capital and operational costs, so that the economic viabilities can attract the interest of private investors. Biological conversion to ethanol of the waste streams produced by the paper and pulp industry is an example where production costs of second generation fuel production was competitive with the equivalent fossil fuel, without any financial grant[23]. Fan and Lynd[23] has shown that such a facility would be competitive with the equivalent fossil fuel price with interest rates above 15% at scales with feed rates as low as 1.1 tons/hr, partly due to annexing the processing plant to an existing pulp mill. Comparing this result to that of Humbird et al.[13], where a 500 MW facility for conversion of untreated lignocellulose to ethanol in a stand-alone facility was not financially competitive against the fossil equivalent at an interest rate of 10%, clearly illustrates the role of feedstock, pre-treatment and processing costs, which were not part of the waste-to-ethanol process. A comparison between a stand-alone facility for second generation ethanol to a facility where second generation ethanol was integrated with sugar syrup fermentation (i.e. first generation bioethanol) demonstrated how the reduction of feedstock costs, sharing of capital equipment and infrastructure improved the Internal Rate of Return (IRR) of the integrated facility by about 7% greater [14].

In South Africa, there are well-established pulp and paper (P&PI) and sugar cane industries (SCCI), and these industries have been identified as opportunities where integration strategies for second generation biofuels may provide the required economic viability. In the P&PI there are opportunities for ethanol production from the Spent Sulphite Liquor (SSL) from a sulphite process, a liquid residue that could provide a low-cost substrate providing fermentable sugars, and opportunities for solid residues such as wood bark to provide process energy and/or feedstock for gasification-synthesis [24]. In the SCCI there are opportunities for co-production of bioethanol from hemicellulose sugars extracted from bagasse and trash[25] with electricity co-generation from the residues, or synthetic fuel production from these feedstocks via gasification-synthesis. Strategies for integrating second generation biofuel production into the P&PI and SCCI face several challenges, as the targeted feedstocks are presently used as sources of process energy, which would otherwise be served by alternative means to secure feedstocks for biofuels production.

Despite the potential technical challenges that must be overcome, there is potential for integration of second generation biofuel production into these two industries, to provide attractive financial returns, through inherent cost-savings associated with integration strategies. Such integration strategies may therefore mitigate the production costs of second generation biofuels and thereby provide opportunities to advance the commercial production of 2G biofuels. Process design for such integration should consider, in addition to economic viability, the existing energy demands of the host facilities where such bioenergy will be integrated, alternative means of maintaining the overall energy balance of the resulting integrated process and securing the net environment benefits to justify biofuels production. This requires comprehensive flow-sheet development and analysis through techno-economic and environmental assessments, both to identify preferred integration strategies and biofuel production methods.

2 Research Problem

The biofuel sector in South Africa has not grown significantly since the introduction of the Industrial Biofuels Strategy in 2007, partly due to insufficient financial incentives to make first generation biofuels production viable, and furthermore, due to the high cost of second generation biofuels production. Attracting private sector investment is a critical requirement to advance the industry, which typically requires an IRR of 25% when selling the fuels at market competitive prices without any government incentives or subsidy. If industrial integration of biofuel production into the P&PI and SCCI is to produce such IRRs to attract investment from the private sector, then there are major challenges that the design of an integrated biofuel processes to overcome.

For the P&PI, challenges include the complications with the fermentation of SSL to ethanol, since these streams have excessively diluted sugar concentrations and have high levels of toxic substances that will inhibit fermentation [26–28]. Furthermore, SSL is currently used to partially fulfil the energy requirements of a P&PI facility[29], and therefore, the production of ethanol will invariably increase the sulphite mill's reliance on external fuel. If a fossil fuel, such as coal, is used to fulfil the additional energy need, then the overall greenhouse gas emissions of the integrated P&PI facility may obliterate the intended environmental benefits of biofuel production and application. This implies that a process design for integrating ethanol production from SSL may need to consider the use of the other biomass residues to sustain the energy needs[30] to maintain the intended net reduction in greenhouse gas emissions in a cost effective manner.

At SCCI's the surplus bagasse residues used for energy co-production, in the form of electricity and/or biofuels, can only be obtained by capital expenditure to improve the energy efficiency of existing sugar mills, thus reducing the process energy requirement for sugar production, while also complementing bagasse supplies with trash residues, collected from agriculture and transported to

the mill. Both bagasse and trash lignocellulose residues require efficient pre-treatment to solubilise the hemicellulose sugars from the lignocellulose matrix, and provide a feedstock for ethanol production, or alternatively, require efficient and cost effective gasification to produce syngas for biofuels synthesis. Furthermore, the biofuel production processes would have to compete for access to available lignocelluloses with highly efficient technologies for electricity generation, such as high pressure efficient boilers or advanced Biomass Integrated Gasification and Combined Cycles (BIGCC) that would generate surplus electricity for export and sales [31–33].

3 Research Question

The question that this research aims to answer is that whether process flow-sheets based on plausible techniques can be developed for efficient integration of second generation biofuel production into the P&PI and SCCI, using residues from these industries, resulting in integrated processes that are technically, economically and environmentally viable and beneficial. Such integration must be technically viable in that the energy requirements of the host industries are not compromised in any significant manner. The technical performances used in these flow-sheets would only be based on published design protocols and measured performances, and would thus be reflective of what is practically achievable. Integrated processes must also be economically viable to yield a minimum IRR of 25% to attract the interest of private investors. Furthermore, the biofuel production and consumption life cycle should be able to maintain a net greenhouse gas reduction, to be environmentally viable and acceptable. Process simulation of flow-sheets, and detailed analysis of the results of simulations for flow-sheet development, was selected as an appropriate methodology to address these requirements.

4 Aims and Objectives

The overall aim of this study is to develop and assess processes for second generation biofuel production that integrate into the existing SCCI's and P&PI of South Africa, to ensure a feasible integration. Feasible integration of biofuel production entails that the energy needs of the host facility should not be compromised in any significant manner, and it should provide an attractive investment opportunity for a private investor, with acceptable environmental benefits in terms of greenhouse gas emissions. The integration of biological and gasification-synthesis production routes for second generation biofuels production was therefore explored as possibilities in achieving this end. These process developments will be based on flow-sheet analyses by means of process simulations, which will explore novel combinations of existing process technologies, heat integration possibilities and optimisation of process conditions. Flow-sheet analyses will also inference the improvements in the performance of processes that will arise with the expected advancements of processing technologies. Based on the outcomes of the various flow-sheet analyses, conclusions will be made regarding the feasibility of the processes developed. Based on the potential bottlenecks that could be identified, recommendations will be made for further investigations.

5 References

[1] Silva V, Rouboa A. Optimizing the gasification operating conditions of forest residues by coupling a two-stage equilibrium model with a response surface methodology. Fuel Process. Technol. 2014;122:163–9.

[2] Guo H, Peng F, Zhang H, Xiong L. Production of hydrogen rich bio-oil derived syngas from co-gasification of bio-oil and waste engine oil as feedstock for lower alcohols synthesis in two-stage bed reactor. International Journal of Hydrogen Energy 2014:1–12.

[3] Luo L, Van de Voet E, Huppes G. Life cycle assessment and life cycle costing of bioethanol from sugarcane in Brazil. Renew. Sustain. Energ. Rev. 2009;13:1613–9.

[4] Gonzalez-Garcı S, Luo L, Moreira MT, Feijoo G, Huppes G. Life cycle assessment of hemp hurds use in second generation ethanol production. Biomass Bioenerg. 2012;36:268–79.

[5] Domac J, Richards K, Risovic S. Socio-economic drivers in implementing bioenergy projects. Biomass Bioenerg. 2005;28:97–106.

[6] Department of Minerals and Energy. Biofuels Industrial Strategy of the Republic of South Africa 2007.

[7] Leibbrandt NH. Techno-Economics Study for Sugarcane Bagasse to Liquid Biofuels in South Africa: A Comparison between Biological and Thermochemical Process Routes. PhD Dissertation Department of Process Engineering. University of Stellenbosch, University of Stellenbosch 2010.

[8] Deenanath ED, Iyuke S, Rumbold K. The Bioethanol Industry in Sub-Saharan Africa : History, Challenges, and Prospects. Journal of Biomedicine and Biotechnology 2012;2012.

[9] Mabee WE, Mcfarlane PN, Saddler JN. Biomass availability for lignocellulosic ethanol production. Biomass Bioenerg. 2011;35:4519–29.

[10] Naylor R., Liska A., Burke M., Falcon W., Gaskell J., Rozelle S., et al. No TitleThe Ripple Effect: Biofuels, Food Security, and the Environment. Science and Policy for Sustainable Development 2011;49:30–43.

[11] Sims REH, Mabee W, Saddler JN, Taylor M. An overview of second generation biofuel technologies. Bioresour. Technol. 2010;101:1570–80.

[12] Wiloso EI, Heijungs R, Snoo GRD. LCA of second generation bioethanol : A review and some issues to be resolved for good LCA practice. Renew. Sustain. Energ. Rev. 2012;16:5295–308.

[13] Humbird D, Davis R, Tao L, Kinchin C, Hsu D, Aden A, et al. Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol. National Renewable Energy Laboratory 2011.

[14] Dias MOS, Junqueira TL, Cavalett O, Cunha MP, Jesus CDF, Rossell CEV, et al. Integrated versus stand-alone second generation ethanol production from sugarcane bagasse and trash. Bioresour. Technol. 2012;103:152–61.

[15] Haarlemmer G, Boissonnet G, Imbach J, Setiera P-A, Peduzzia E. Environmental Science Second generation BtL type biofuels – a production cost analysis. Energy and Environmental Science 2012;5:8445–56.

[16] Seabra JEA, Tao L, Chum HL, Macedo IC. A techno-economic evaluation of the effects of centralized cellulosic ethanol and co-products refinery options with sugarcane mill clustering. Biomass Bioenerg. 2010;34:1065–78.

[17] Huang H-jiang, Ramaswamy S, Al-dajani W, Tschirner U, Cairncross RA. Effect of biomass species and plant size on cellulosic ethanol : A comparative process and economic analysis. Biomass Bioenerg. 2009;33:234–46.

[18] Hamelinck C., Faaij AP. Outlook for advanced biofuels. Energ. Policy 2006;34:3268–83.

[19] Anex RP, Aden A, Kabir F, Fortman J, Swanson RM, Wright MM, et al. Techno-economic comparison of biomass-to-transportation fuels via pyrolysis , gasification , and biochemical pathways. Fuel 2010;89:S29–S35.

[20] Vohra M, Manwar J, Manmode R, Padgilwar S, Patil S. Journal of Environmental Chemical Engineering Bioethanol production : Feedstock and current technologies. Biochemical Pharmacology 2014;2:573–84.

[21] Kazi FK, Fortman JA, Anex RP, Hsu DD, Aden A, Dutta A, et al. Techno-economic comparison of process technologies for biochemical ethanol production from corn stover q. Fuel 2010;89:S20–S28.

[22] Klein-Marcuschamer D, Oleskowicz-popiel P, Simmons BA, Blanch HW. The Challenge of Enzyme Cost in the Production of Lignocellulosic Biofuels. Biotechnology and Bioengineering 2012;xxx:1–5.

[23] Fan Z, Lynd ÆLR. Conversion of paper sludge to ethanol , II : process design and economic analysis 2007:35–45.

[24] Isaksson J, Pettersson K, Mahmoudkhani M, Åsblad A, Berntsson T. Integration of biomass gasification with a Scandinavian mechanical pulp and paper mill – Consequences for mass and energy balances and global CO2 emissions. Energy 2012;44:420–8.

[25] Purchase BBS, Walford SN, Waugh EJ. AN UPDATE ON PROGRESS IN THE PRODUCTION OF ETHANOL FROM BAGASSE. Proceedings a/The SouthAfrican Sugar Technologists' Association - June 1986 1986:33–6.

[26] Marques AP, Evtuguin DV, Magina S, Amado L, Prates A. Composition of Spent Liquors from Acidic Magnesium – Based Sulphite Pulping of Eucalyptus globulus. Journal of Wood Chemistry and Technology 2009:37–41.

[27] Nigam JN. Ethanol production from hardwood spent sulfite liquor using an adapted strain of Pichia stipitis. Journal of Biotechnology 2001;26:145–50.

[28] Bajwa PK, Shireen T, Aoust D, Pinel D, Martin VJJ, Trevors JT, et al. Mutants of the Pentose-Fermenting Yeast Pichia stipitis With Improved Tolerance to Inhibitors in Hardwood Spent Sulfite Liquor. Biotechnology and Bioengineering 2009;104:892–900.

[29] U.S. Environmental Protection Agency. Available and Emerging Technologies for Reducing Greenhouse Gas Emissions from the Pulp and Paper Manufacturing Industry. North Carolina: 2010.

[30] Huang H-jiang, Ramaswamy S, Al-dajani WW, Tschirner U. Process modeling and analysis of pulp mill-based integrated biorefinery with hemicellulose pre-extraction for ethanol production : A comparative study. Bioresour. Technol. 2010;101:624–31.

[31] Wienese A. Boilers, boiler fuel and boiler efficiency. Proceedings: The South African Sugar Technologists' Association 75, 2001, pp. 275–81.

[32] Ensinas AV, Nebra SA, Lozano MA, Serra LM. Analysis of process steam demand reduction and electricity generation in sugar and ethanol production from sugarcane. Energy Conversion and Management 2007;48:2978–87.

[33] Nsaful F. PROCESS MODELLING OF SUGAR MILL BIOMASS TO ENERGY CONVERSION PROCESSES AND ENERGY INTEGRATION OF PYROLYSIS. Stellenbosch University, 2012.

Chapter 2: Literature Review

1 Second Generation Biofuel Processes

In this section, the technical and economic characteristics of the processes for second generation biofuels production are discussed. Firstly, a brief overview of the production process of bioethanol and synthetic fuels from lignocellulosic biomass is presented, followed by a discussion on the current economic status of stand-alone production plants. Thereafter, a discussion of the key technologies used in the second generation processes and the possible variations will be given.

1.1 General technological Overview

The process flow depicted in Figure 1A for the "stand alone" bioethanol production process through hydrolysis and fermentation shows that biomass is initially pre-treated to solubilise hemicellulose fractions and to disintegrate the structure of the cellulose fraction[1,2]. If the biomass is received in large particle sizes, size reduction via comminution methods, such as chipping or slashing, is necessary prior to pre-treatment[1]. The performance of a bioethanol process is largely dependent on the efficiency of pre-treatment, as pre-treatment itself is energy intensive, and because the downstream processes are directly dependent on the characteristics of the pre-treated slurry[3,4].

The pre-treatment slurry is then hydrolysed in the presence of enzymes in order to decompose the cellulose into glucose and the sugars are then fermented to ethanol by microbes, and the ethanol is separated from the unconverted sugars[1]. The hydrolysis and fermentation can either be configured as an integrated process, i.e. simultaneous saccharification and fermentation (SSF) or as dedicated processes, I.e. separate hydrolysis and fermentation (SHF). The former lends advantages in terms of reduced process costs and an improved selectivity to the hemicellulose sugars, while the

latter lends advantages to individual optimisation[4]. Irrespective of the mode of hexose sugar processing, the enzymatic hydrolysis remains a crucial aspect of the economic potential of bioethanol processes, as obtaining enzymes bears a significant process cost[5]. The unconverted sugars, cellulose and lignin fraction are then converted to heat and power via combustion methods[1,2]. The typical "stand alone" process for ethanol production from lignocellulose is characterised by extensive conversion of all sugars in the raw material to ethanol, and being a self-sufficient process that is not integrated with or dependent on any adjacent industrial facilities.

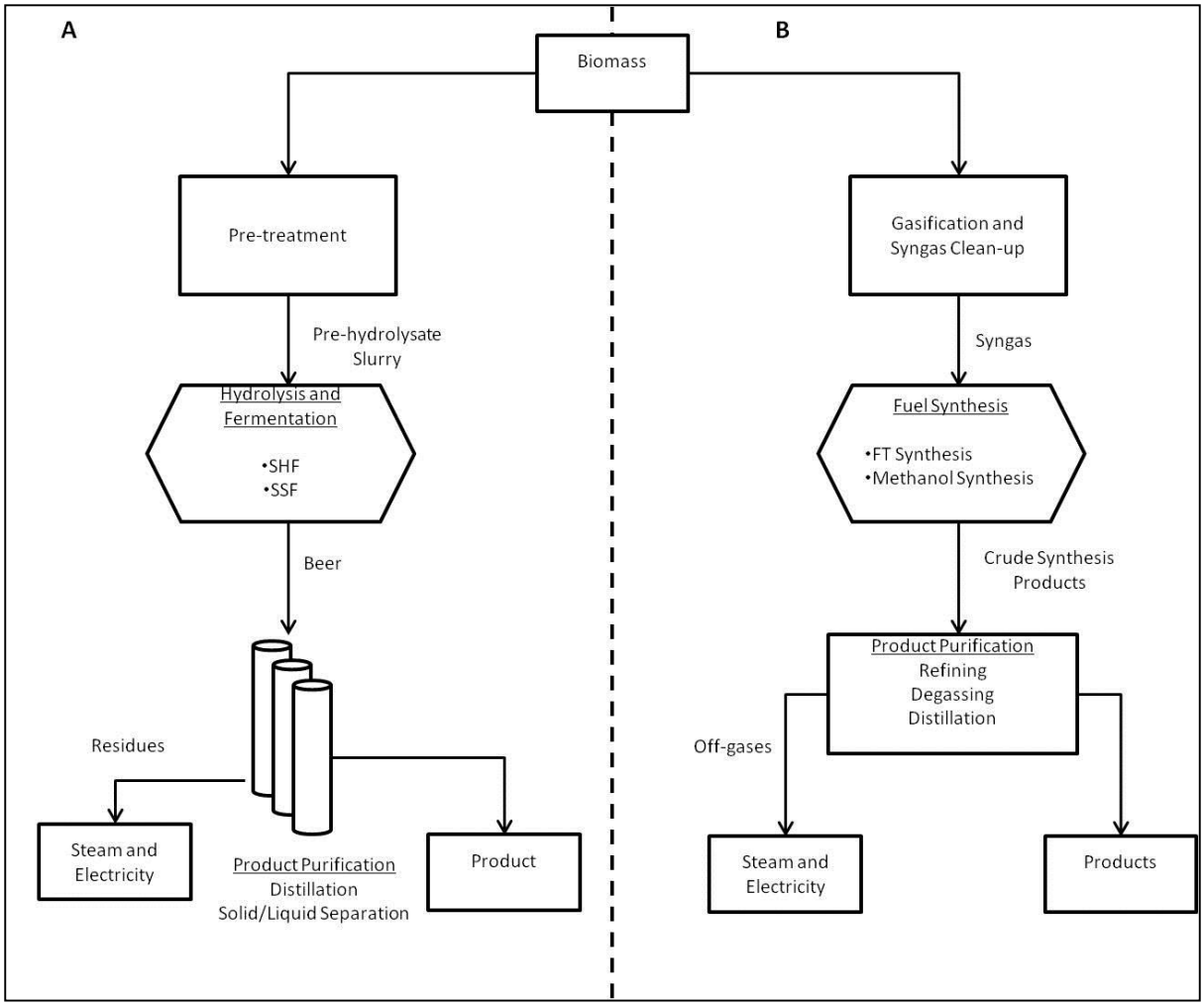


Figure 1: Overview of (A) Second Generation Bioethanol through Fermentation and (B) Gasification-synthesis process

The gasification-synthesis process for synthetic fuel production (Figure 1.B) [4,6–8] typically begins with particle size reduction, followed by biomass drying, which is typically achieved with waste heat generated by the process. Biomass that is obtained as small particles, such as sugarcane bagasse is typically dried without any further size reduction. The dried, fine biomass is then converted to synthesis gas (syngas) via gasification and the resulting syngas is purified and conditioned to remove acidic gasses such as carbon dioxide and hydrogen sulphide. The efficacy with which purified, compressed syngas is generated from biomass is an important parameter in the gasification-synthesis process, as the major processing costs are concentrated in that area[9,10]. The syngas is then converted to a crude oil through the chemical synthesis process, which is dehydrated and refined, or methanol which is purified via distillation. The unconverted syngas is separated from the synthetic products and converted to heat and power.

1.2 Overview of the economic status of 'stand-alone' facilities for second generation biofuels production

A brief survey of the economic findings from recent literature on "stand-alone" second generation studies in shown in Table 1. These results are summarised as the scale of production, expressed as the calorific value of the biomass input (MW_{th}), based on the Higher Heating Value (HHV), the minimum fuel selling price (MFSP) and IRRs at which the project in the studies were evaluated. As a reference point, the competitive selling price of the fossil fuel equivalent is shown, as well as the interest rate charged of the loan from the banks. As the IRRs listed tend towards the values of the interest rates, rather than the high returns of private investors typically characterised by an IRR of 25%[11], then these investments are reflective of low equity-to-debt financing agreements and thus, the low IRRs are indicative of a low potential to attract investment. Furthermore, the values of these parameters that characterise a feasible investment in a South African context are also shown. The fossil equivalent for the bioethanol price represents the price of an equivalent amount of gasoline in the geographical context of the study, based on the difference in energy content. For

the gasification-synthesis, the equivalent price was that of FT diesel in the European context, as reported by Caula[12] while the equivalent price in the context of the USA quoted by Liu et al[13] was the levelised cost of FT fuels based on the oil price of 75$ per barrel, that was concurrent with that study.

Table 1: Survey of Economic Outcomes from Recent Literature (all data adjusted to 2012 US$)

	Scale	MFSP	Project IRR	Competitive Selling Price	Interest Rate
	MW_{th}	$/l	%	$/l	
Second generation Bioethanol					
Humbird et al[1] (USA)	500	0.75	10%	0.52	8%
Kazi et al[14] (USA)	500	1.19	10%	0.52	8%
Laser et al [15]	920	0.28	12%	0.52	8%
Parameters for a South African Context	600	0.53			11.5%
Gasification-synthesis Routes					
Haarlemeer et al[16]	400	1.43		0.53	7%
Liu et al[13]	500	1.41	14%	0.81	7%
Caula[12]	1000	1.17	12%	0.53	5%
Parameters for a South African Context	600			0.76	11%

It is generally seen that the selling prices of the fuel required for bioethanol process routes at a processing scale of 500MW ranged from 0.74-1.17 US$/l for satisfying an IRR of 10% in the context of the USA. These selling prices however, are all above the competitive price of the equivalent fossil fuel, which shows that they were not economically favourable. Outcomes that are favourable are shown by Laser et al[15] who considered the Consolidated Bio-Processing technology that marks the technological endpoint of the second generation bioethanol processing route (i.e. the best possible anticipated performance of future production facilities, when all technological development has been completed), as CBP avoids enzyme costs and assumes high (>90%) conversions of raw materials

to products. The economic status acquired for the gasification-synthesis processes in European contexts are shown to range from the more favourable outcomes where selling prices of FT fuels are 1.17 US$/l for satisfying interest rates of 12% to more pessimistic indications that show that selling prices as high as 1.43 US$/l are required to satisfy the interest rate of 7% that is typically charged by a bank. The outcomes by Caula[12] are more favourable than the rest, possibly due to the processing scale of a 1000MW that was considered, thus demonstrating an effect of plant scale on economic potential. Generally, gasification-synthesis processes in European contexts were not economically viable, since the minimum selling price of the FT fuels exceeded the fossil equivalent by more than 2 fold.

In a study relating to the South African context [10], the IRR that was measured for the second generation bioethanol and gasification-synthesis routes were 13.3 and 10.2% respectively, using the fuel selling prices shown in Table 1 in addition to a government subsidy. The cost of enzymes in the bioethanol route was estimated at 0.26 U$ per gallon ethanol, which was not realistic and therefore, a corrected IRR based on a more realistic enzyme cost of 0.45 U$/gal[1] was estimated at 9.7%. Thus, it was shown that the IRRs were less than the South African commercial interest rates of 11-12%, which meant that these investments would not even be feasible for capital pools characterised by high debt-to-equity ratios. Considering this study[10], and the values and conclusions drawn from Table 1, it can be concluded that the stand alone second generation projects in their current technological state are largely still uncompetitive from an investment perspective, especially without extensive financial support from government.

1.3 OVERVIEW OF ALTERNATIVE TECHNOLOGIES FOR SECOND GENERATION BIOETHANOL PRODUCTION

1.3.1 Fermentation of Hemicellulose Substrates to bio-ethanol

As the enzymes required to convert the cellulose fractions to ethanol impose a major cost, converting only the hemicellulose component of lignocellulose to ethanol, which are more readily available for hydrolysis than sugars in cellulose, could offer an advantage in terms of reducing process costs. In this section, the fermentation of two types of hemicellulose substrates will be discussed, (i) hemicellulose hydrolysates originating from lignocellulose via a pre-treatment/fractionation step and (ii), the hemicellulose sugars available in SSL.

Hemicellulose hydrolysis through lignocellulose pre-treatment and fermentation of liberated sugars

Given that the hemicelluloses sugars comprise between 26-35% of lignocellulosic biomass residues at sugar cane crushing industries (SCCI)[17,18], the co-production of bioethanol and electricity seems highly plausible if the bagasse is initially fractionated to produce a hemicellulose sugar rich stream, prior to conversion of solid residues to electricity. This required that the SCCI facility itself is energy efficient, so as to maximise the availability of bagasse raw materials for production of exportable energy products. One typical method for hemicelluloses extraction from lignocellulose for recovery of fermentable (monomeric) sugars is dilute acid treatment in liquid hot water. Aguilar et al[19] showed with this method that yields of monomeric sugars of 92% are possible at an acid concentration of 2%, but this conversion was achieved at a solids content of only 10% by mass, resulting in diluted sugar product streams. Similarly, Jeevan et al[20] demonstrated that although a yield of 80% of monomeric sugars was possible at 10% WIS, it dropped significantly at higher solids contents. High yields at higher solid loadings are possible, though higher acid concentrations are required, which could result in sugar degradation. Paiva et al[21] had sugar yields of 96% at an acid concentration of 3.10%, when the solid content was 16.7%. The implication of dilute conditions is

that there would be intensive energy demands in the process that uses this method, since the concentration of sugars in the hydrolysate would be low.

Steam explosion with sulphur dioxide is an alternative method of liberating hemicelluloses sugars at high solid concentrations[22,23], which implies greater sugar concentrations in the hydrolysate, with less energy demands for downstream concentration steps. In the evaluations of full scale second generation applications , where steam explosion and dilute acid have been compared as alternative pre-treatment techniques[2], steam explosion was a more energy efficient method than dilute acid, because a significant amount of externally supplied energy was needed to supplement the energy demands caused by dilution effects. It should be noted that the only available energy from the feedstock in these setups were the lignin and fractions of unconverted carbohydrates. It is not expected that these limitations would apply to a scenario where the lignin and the entire cellulose fraction is available for heat and electricity production.

With regards to the fermentation of acid or steam explosion hydrolysates, there has been a considerable success in developing microbial strains with this capability[24] and the technology has been successfully demonstrated on a laboratory scale. Hemicellulose hydrolysates primarily contain pentose sugars, e.g. xylose and arabinose, with limited amounts of glucose, as well as a range of sugar degradation products from pre-treatment, which are inhibitory to fermentative processes. Fermentative organisms capable of efficient pentose conversion to ethanol, in the presence of these inhibitors, are therefore required[22,25,27] . Using an adapted strain of the *Pichia Stipitis* yeast that ferments pentose in its native state, Kurian et al[25] obtained a yield of 82.5% ethanol from a hemicellulose hydrolysate derived from sorghum bagasse that contained 92g/l of sugars, while Nigam et al[26] obtained an ethanol yield of 80.0% from an acid hydrolysate derived from wheat straw, containing 80g/l sugars. Robust recombinant strains of *Saccharomyces cerevisiae,* such as

TMB400, have been used to convert 85% of the pentose in toxic environments during simultaneous saccharification and fermentation [27]. More recently, the NREL converted 92% of hemicellulose sugars in a non-detoxified enzymatic hydrolysate that had a total sugar concentration of about 150 g/l, using the *Zymomonas mobilis* strain of Du Pont[28].

Fermentation of Hemicellulose Sugars present in Spent Sulphite Liquor from Sulphite Pulping

Experimental work in literature on SSL fermentation is numerous, such as the study of Bjorling and Lindman[29] who considered softwood SSL that had a predominance of hexose sugars, and Nigam[30] that considered hardwood SSL that had a predominance of pentose sugars. Ethanol yields of 75.6 $\pm$4.5% based on the initial mass of total dissolved sugars in the effluent stream were typically attained with yeasts that were capable of fermenting xylose (pentose sugar). In all cases, the SSL contained high amounts of lignocellulose degradation products such as phenolic compounds and acetic acid that is generated by the pulping process, and these are inhibitory to fermenting yeasts[30–32]. One method of minimising the effects of the degradation products was to steam strip the excess SO_2 present in SSL, and then to add lime to bring the pH to 5 [29]. Furthermore, alkaline detoxification by raising the pH to 9-10 to deactivate the inhibitors was shown by Helle et al[33] to improve the yield of ethanol by 27%, while Nigam[30] had shown that the fermentability of liquor treated with alkaline detoxification improved by 25%.

In another study by Helle et al[31], a recombinant strain of *Saccharomyces cerevisiae 259ST* resulted in conversions of 75 and 85% of the sugars in magnesium oxide based SSL derived from hardwood that was concentrated at 30 and 20% solids concentration, without any detoxification. Thus, these results imply that detoxification may only serve as a conservative measure when a robust recombinant strain is used. Additionally, it was shown that the yeast cells were inhibited by osmotic stress when the concentration of solid material was too high. It is seen that even though the lower

yield occurred at high (85%) substrate concentrations, the beer product had a higher concentration of ethanol. This implies there would be a trade-off between systems with lower and higher ethanol yields in a flow sheet setup, as the energy costs associated with the distillation and purification would be higher with the 20% solid concentration.

Producing bioethanol from SSL is an established industrial process, as the Borregaard mill in Norway has been producing bioethanol from SSL generated from softwood at a rate 20 million litres per annum[34], while the Tembec sulphite mill in Canada produces bioethanol at a rate of 18 million tons per annum[35]. The hemicellulose substrates in such softwoods is predominated by hexose sugars, and thus, fermentation by conventional industrial yeasts was readily done[31]. In hardwood pulping processes such as South Africa, however, hemicellulose substrates will be dominated by pentose sugars and thus, ethanol production only becomes feasible if strains capable of fermenting pentose sugars are used [27,31,33]. Recombinant strains of *Saccharomyces cerevisiae* that are genetically modified to ferment pentose sugars are preferable to native strains that ferments pentose sugars, such as *Pichia stipitis*, as the latter tends to metabolise ethanol[26,30]. The recombinant strains used has also shown to be robust to the presence of compounds such as phenolics and organic acids that are inhibitory to microbial activity. These compounds were often found in SSL at significant concentrations [30,31,33].

1.4 Overview of process technology in Methanol or FT syncrude production via Biomass Gasification and Synthesis

Gasification-synthesis processes have two primary processing stages, which are (i) the conversion of biomass to clean, compressed syngas and (ii), the conversion of the syngas to a synthetic liquid product. In this section, the various technologies available for the two processing stages are discussed.

1.4.1 Biomass Gasification

Designs for the gasification of biomass tend to focus on fluidised bed gasifiers for lignocellulosic biomass[36,37], some of which are operated in autothermal gasification (AUT-G) mode, where the gasification medium includes both steam and an oxidant in sub-stoichiometric proportions, to initiate the combustion reactions to supply the reaction heat required by the endothermic gasification (reduction) reactions[38,39]. If a high calorific value of the synthesis gas (syngas) is desired for purpose of Fischer-Tropsch synthesis, then the oxidant is required as pure oxygen that is obtained by an Air Separation Unit, which bears substantial energy and capital costs[7,40]. AUT-G systems can also be pressurised to prevent the costs of the compression of syngas further downstream[8,41], though it requires higher gasifier capital cost[42] and reduces the content of hydrogen and carbon monoxide in the syngas[41]. Fluidised bed gasifiers can also be operated in allothermal gasification (ALO-G) mode, where the gasification agent consists only of steam, to generate a syngas with a calorific value similar to that of the oxygen-fed autothermal systems[40,43]. In the ALO-G system the energy required for the endothermic steam gasification reactions is supplied by a heat transfer medium from an external heat generating source, such as the combustion heat from a fuel and char burner[40,44]. This however, can have a substantial effect of the overall efficiency with which the biomass is converted, notwithstanding the additional capital required for the combustor[40,44].

As syngas production (Figure 2) bears the primary energy and capitals costs in a gasification-synthesis process [9], previous studies have studied the effects of the gasification operating parameters, such as moisture content, temperature, steam-to-biomass ratio (SBR), equivalence ratio (ER) and pressure on the syngas composition and the energy requirements[9,37,44]. The primary predictive tool utilised in such parametric orientated studies is Equilibrium (or Thermodynamic)

Modelling, which has the basic assertion that the composition of the syngas leaving the gasifier unit is similar, or very close to the composition predicted through thermodynamic calculations under equilibrium conditions. This assertion however, bears significant inaccuracies at temperatures of 750-1000^{o}C, which are typical for the gasification of biomass in a CFB[40,45]. This is primarily due to the incomplete cracking of tars and the slow kinetic rate of the reaction of reforming methane with steam at these temperatures [40,45]. However, the application of equilibrium modelling for biomass/derivative gasification at temperatures of 800-1000^{o}C is readily justifiable when a gasification or steam reforming catalyst (such as dolomite or nickel-based), which promotes syngas compositions that are very close to equilibrium and reduces the tar content to acceptable levels [38,46,47], are considered.

The impact of the operating parameters on the gasification performance, predicted with the aid of equilibrium models, is typically evaluated with the gasification efficiency – a term that has slight variances in its definition, depending on the system under consideration[9,40,48]. Schuster et al[40] for example, defined the chemical (gasification) efficiency as the ratio of the flow of calorific energy of the syngas (*numerator*)to the flow of calorific energy in the biomass feed and the steam enthalpy (*denominator*). Leibbrandt et al[9]. defined the gasification efficiency for an oxygen-fed autothermal system similar to Schuster et al[40], but also included the energy costs of producing pure oxygen in the denominator. The gasification efficiency was used by Leibbrandt et al[9] as an optimisation variable in a statistical model, to determine the preferred operating conditions for producing a synthesis gas from sugar cane bagasse (and its pyrolysis products). The target syngas composition contained hydrogen (H_2) and carbon monoxide (CO) at a ratio of 2 for Fischer-Tropsch synthesis. A similar approach where the capabilities of equilibrium models was combined with a statistical model was developed Silva and Rouboa[48], where the operating conditions for producing a H_2 rich product stream from forest residues was found by optimising the cold gas efficiency.

Previous reports on the gasification efficiency, as determined from equilibrium modelling, did not include the impacts of the energy recovery units (such as the steam generator) and clean-up units (such as the Rectisol, see Figure 2) in the definition of gasification efficiency. These additional energy components are affected by the energy balance and operating parameters of the gasifier, as noted by the work by Van der Meijden et al.[49], whom compared various synthetic natural gas (SNG) production systems, defined by the mode of gasification. The steam generating capacity of the unit that cools the synthesis gas (syn-cool generator) is dependent on the enthalpy of the product gas[7,10], which in turn is dependent on the temperature of the gasifier and the flow of gasification medium. Furthermore, the energy demands of the Rectisol unit for syngas clean-up are dependent on the content of acid gases (primarily carbon dioxide (CO_2) and hydrogen sulphide (H_2S)) in the syngas[7,50], which in turn affected by the SBR, ER and moisture[36,40,51]. Thus, the overall efficiency of a synthesis gas production should be inclusive of the energy effects of the downstream units, up to the Rectisol unit. This gives a comprehensive view on the gasification efficiency in response to variations in the gasification operating conditions.

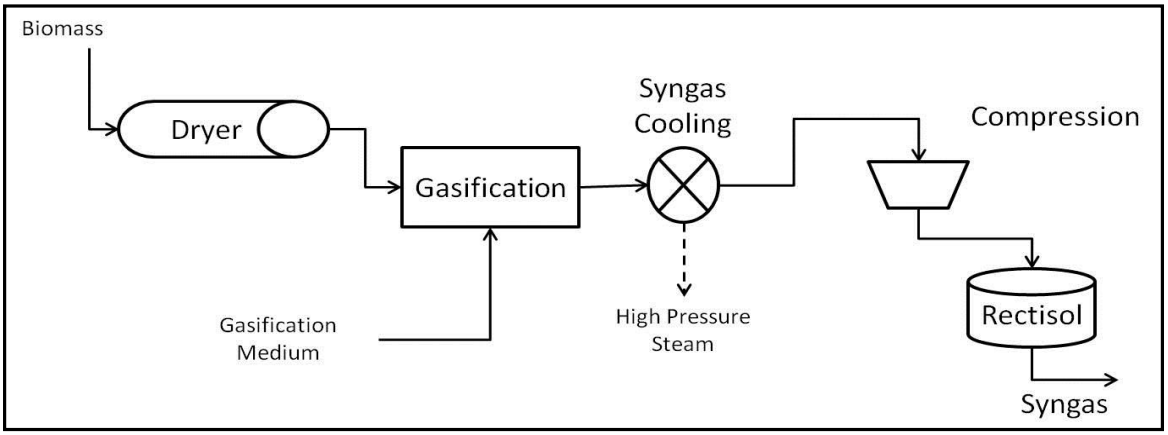


Figure 2: Generic Flow-sheet of Syngas Generation

Selecting a process technology, or set of operating conditions, for gasification based solely on a measure of energy efficiency does not account for the economics of variable capital and operating costs, incurred by changes in operating conditions [52,53]. Generally speaking, processing units that

are more efficient at generating energy (and consuming energy), have greater capital and operational costs, compared to less efficient counterparts[52,53]. As an example, oxygen-fed autothermal gasification has higher conversion efficiency than an allothermal system, since the entire amount of biomass fed is used to produce syngas[39]. However, AUT-G systems that are oxygen blown, involve significant operating and capital expenditure, due to production of pure oxygen[40,44], thus indicating a trade-off between costs of efficiency. Thus, the optimisation of a gasification system should also aim to minimise the overall costs of producing syngas by accounting for both the capital and operational cost implications for the overall syngas production train, up to purified syngas suitable for synthesis, when varying the operating conditions.

1.4.2 Methanol Synthesis

The Conventional synthesis configuration for methanol entails a fixed bed gas phase reactor, with copper/zinc/aluminium catalyst [54,55] that sinters with rapid temperature increases due to the exothermic methanol synthesis reactions. Thus, heat is removed from the reactor by employing a high recycle ratio of about 5:1 (mol flow mixed feed/fresh feed) of the un-reacted gases[55], in order to limit the conversion of the syngas to 30% per pass. The high recycle ratios however, bears significant capital and operational costs because the recycle stream must be recompressed[55].

The Advanced methanol synthesis reactors are operated with the catalyst suspended in an inert liquid medium through which the syngas is bubbled[55,56]. Synthesis gas then defuses through the liquid to the catalyst to react, and the reaction product diffuses form the catalyst surface into the gas phase. The liquid medium also enables a rapid transfer of the reaction heat from the reaction surface to a cooling medium, such as steam generated in a coil. This enables conversions of about 70%[55] without any concern about the catalysts sintering.

1.4.3 Fischer-Tropsch (FT) synthesis

The principle differences between Conventional and Advanced synthesis configurations for FT liquid synthesis from syngas are similar to those described for methanol synthesis, in that conversion of syngas in a conventional fixed bed FT reactor is limited to about 40% per pass, to prevent the heat from the exothermic synthesis reactions from sintering the catalyst[6,57]. High recycle ratios of the un-reacted gases of about 3:1 (mol flow mixed feed/fresh feed) are employed in order to purge the reaction heat, in addition to improving the overall FT product yield. In the case for Conventional FT synthesis, however, the costs are accentuated by the compression of the recycle gas and the subsequent reforming of the light hydrocarbon gases (C_1-C_4) to CO and H_2 in an Auto-Thermal Reformer (ATR) [7].

Similar to Advanced methanol synthesis configurations, the Advanced FT synthesis reactors also operate in liquid phase created by an elevated pressure, to ensure that the wax products are condensed. The catalyst is suspended in the liquid wax, which trickles down and is removed from the bottom of the reactor[6,57]. Thus, reaction heat is rapidly transferred through the liquid to cooling coils and syngas conversion can go up to 90% per pass [57,58].

Two operating schemes normally applied for FT synthesis are high temperature (HTFT) which operates at 300-350^{o}C and low temperature (LTFT) in the range of 200-250^{o}C [57,58], for either the conventional or advanced reactor concepts. Low temperature (LTFT) processes tends to generate products with high molecular weights and HTFT produces molecular weights that are mostly in the gasoline range. While the product of the former requires cracking at a refinery, it is stable[58], unlike the product of the HTFT which contains significant amounts oxygenates that destabilizes the synthetic crude, making hydrogenation of the product a necessary step for stabilization[59]. Thus

LTFT would be suitable for bio-syncrude production, as it was seen in Consonni et al[59] that hydro-treating introduced more costs.

2 Overview of the Cane Crushing and Paper and Pulp Industries and the use of residues

2.1 Sugar Cane Crushing Industry

Sugarcane Crushing Industries (SCCI) are represented by Autonomous Ethanol Distilleries and Raw Sugar Industries, and a conceptual process flow diagram of a typical sugar mill in the Raw Sugar Industry (RSI), which is largely representative of the SSCI in South Africa, is shown in Figure 3. There are currently 14 mills in South Africa and the average size of the mills is a processing capacity of 300 tons of wet cane per hour. The cane is washed to remove the impurities before it undergoes size reduction with cutting knives, which are typically driven by steam in the South African context[60,61]. The sugar is then extracted from the cane particles, either by a crushing system, or by a diffuser. In the South African sugar mills, diffusers are mostly used, since they are more energy efficient than the milling system[62,63]. The juice then undergoes clarification with lime addition, to remove all solid impurities and then concentrated from a concentration of 15% solids to produce a concentrate of about 65% in a series of multi-effect evaporators, which in South Africa, operate with 5 or 4 effects[64]. The concentrate then enters the crystallisation units to generate raw sugar crystals in the vacuum pans, which are heated using the vapour that is bled from the multi-effect evaporators[64,65]. The crude product from the crystallisation unit is separated into molasses and crystals and the crystals are dried using exhaust steam[60,63].

Older sugarcane mills that are less energy efficient will typically demand 0.55 tons of steam for every wet ton of cane (WTC) processed[60]. Modifications and modernisation of energy utilisation in sugar mills, which require significant capital investments, could lead to more efficient energy usage, with specific steam demands as low as 0.28 ton/WTC in the long term[60,66], while a mid-term target for

the steam consumption is estimated at 0.40 ton per WTC[64]. The mid-term goal of 0.40 ton per WTC is the maximum permitted steam usage if the mill is to be considered as a platform for exporting renewable energy[64]. Modifying the sugar mill to reduce the steam demand from 0.55 to 0.40 ton per WTC, for the purpose of making surplus bagasse available export to energy-producing facilities, includes the following technical measures:

- Optimising imbibitions rate to reduce the amount of evaporation needed[64].
- Convert from the batch pans to continuous pans, and reduce the pan movement water[61,64,65].
- Use a 5 effect evaporator where vapour is bled to the vacuum pans at a lower effect[65].
- Optimise the flashing of condensates for steam recovery[64].
- Electrify the turbine drivers[61,67].

These modifications will entail an investment cost that is estimated at US$ 17.32 million[61,64] (all currency quoted in $2012) for the average size mill in South Africa, which crushes 300 ton WTC per hour[64].

A typical representative sugarcane mill generates about 0.30 tons of bagasse per ton of sugar cane processed[68]. The post-harvesting residues of sugarcane (trash), can typically be generated at a yield of 1.16kg for every kilogram of bagasse generated[69]. Currently, bagasse is inefficiently converted to heat and electricity by means of a low pressure boiler ranging from 15-22 bar[60,65], with some electricity available for export, depending on the efficiency of the mill, while the trash is left on the field. This steam is then expanded with turbines to 4 bar[70] to generate electricity that is sufficient for the mill and a minor amount for export.

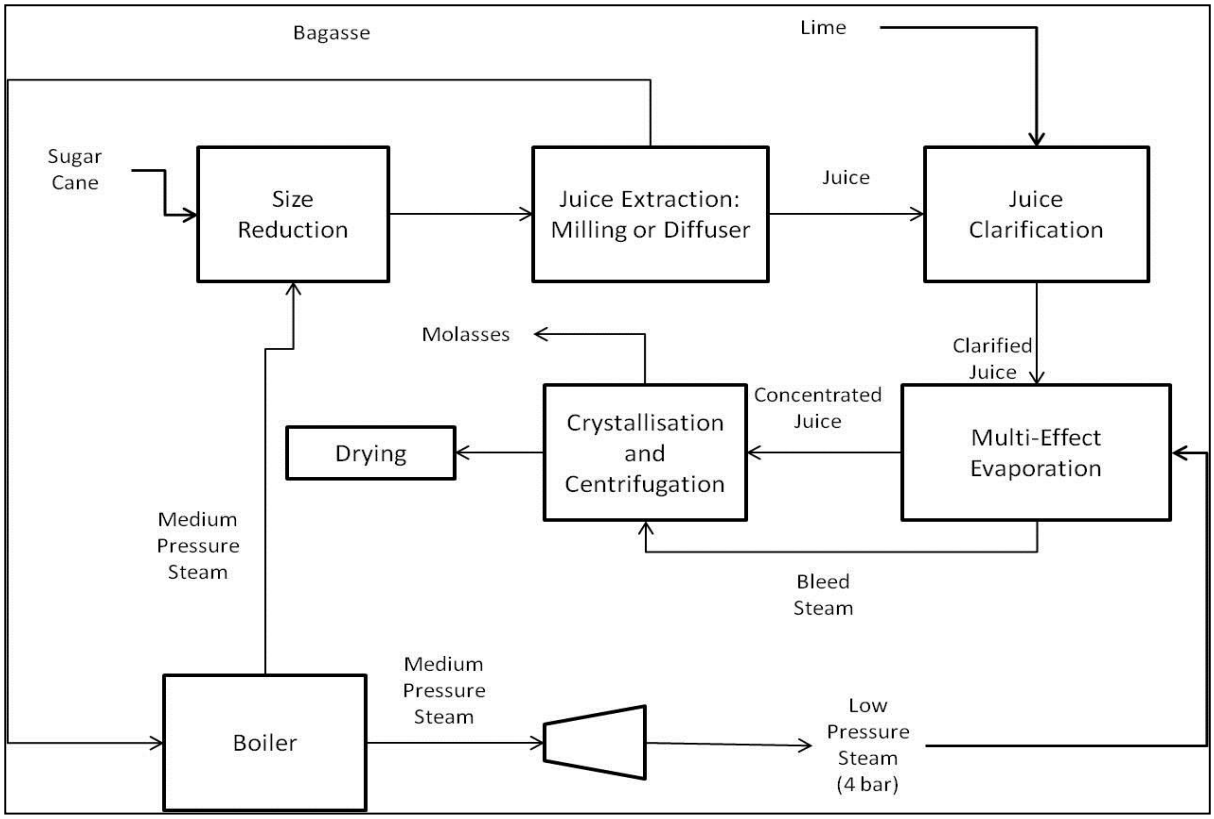


Figure 3: Process Flow Diagram of a Sugar Mill

2.2 PULP AND PAPER MILLS

Paper and pulp industries (P&PI) includes the Sulphite and Kraft Processes, and these generate onsite residues that include the bark that is generated when the logs are debarked and the liquid residues generated by the digestion of the wood chips[71]. In sulphite pulping processes the liquid residue is referred to as Spent Sulphite Liquor (SSL) [34], whereas the liquid residue from Kraft and alkaline pulping of lignocellulose is known as Black Liquor. In the South African P&PI, the Sulphite pulping process is primarily applied for the production of chemical cellulose, which is therefore the focus of the present study. As an industrial context for this study, the Saiccor facility at Umkomaas, KZN would be considered, which currently processes 8000 tons per day of *Eucalyptus Globulus* hardwood.

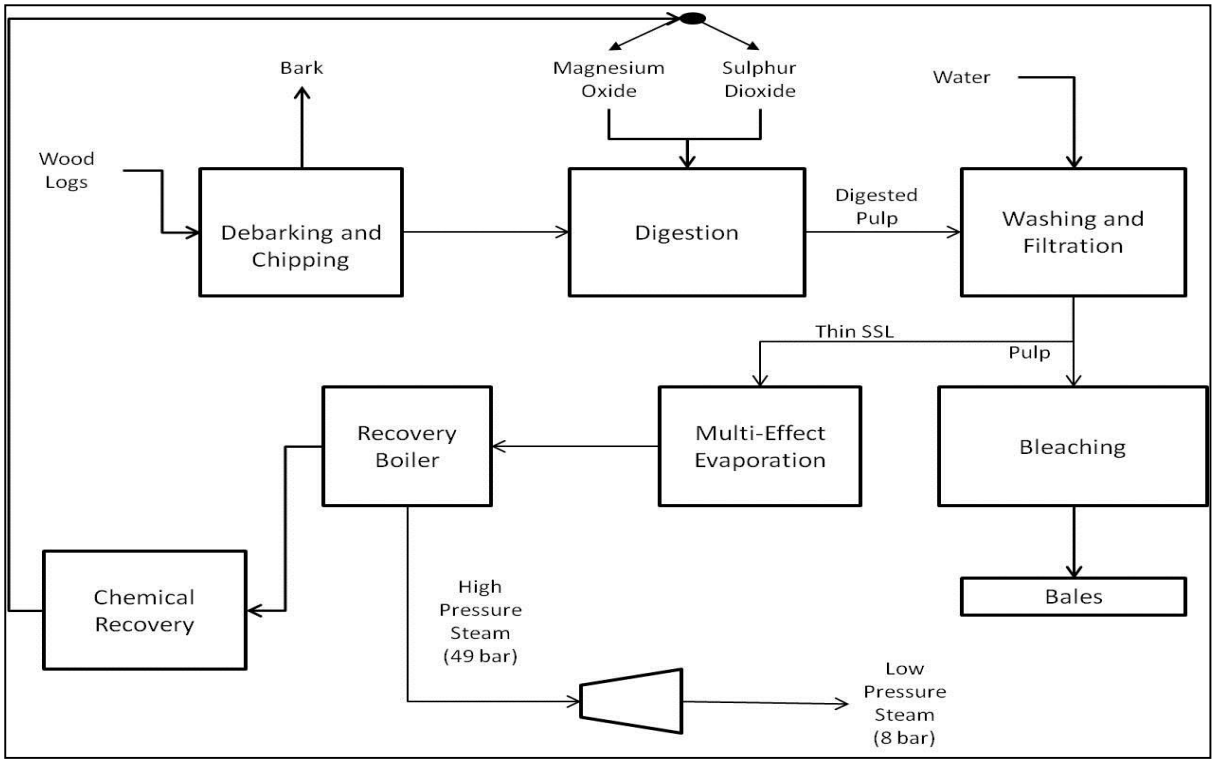


Figure 4: Process Flow Diagram of a Spent Sulphite Process in South Africa

An overview of the Sulphite Process is shown in Figure 4, where wood is firstly debarked and then chipped. The wood chips are then mixed with water and enter the digester to remove the hemicellulose and lignin through solubilisation[72]. The solubilisation occurs at a temperature of approx. 160^{o}C with sulphur dioxide in combination with either magnesium oxide (Mg-O) or calcium oxide (Ca-O). Currently, the Saiccor facility has three digestion lines, two of which use Mg-O as the solubilisation agent while the third utilises Ca-O. The digester product slurry is then washed and separated into the pulp, which is bleached and rolled into sheets, and diluted SSL, which contains lignosulphonates (water-soluble lignins), sugars and organic acids and phenolic compounds[73]. The SSL from the Mg-O lines is processed for the recovery of energy (steam and power) and pulping chemicals, by concentrating the SSL in a multi-effect evaporator prior to combustion of the resulting syrup in a recovery boiler, which recovers magnesium oxide and sulphur dioxide for digestion process [74]. The energy generated from the combustion of SSL is often not sufficient to satisfy the energy demands of the mill itself, and an additional fuel source such as bark, field biomass residues

(collected and processed into hog fuel) or coal is needed [71,74]. The SSL from the Ca-O digestion at Saiccor is split into two streams, one of which is sent to a neighbouring lignosulphonates recovery plant, and the second is discharged as effluent.

2.3 Advanced Electricity Generation from Biomass Residues

The efficient and cost effective conversion of biomass to electricity is paramount to promoting the generation of heat and power from renewable resources. Biofuel production from lignocellulose is also frequently associated with co-generation of surplus electricity, for export to the grid. In this section, competing technologies for efficient conversion of biomass residues to electricity are discussed. Such technologies apply to both fresh biomass and solid residues from biomass processing, available from biofuel production, such as pre-treatment residue, the solid components in fermentation residue or supplementary bio-wastes.

Newer systems for generating electricity from biomass utilise boilers that operate at medium-to-high pressures (45-105 bar), which result in greater generation of electricity [60,67,70,75] when compared to the low-pressure systems (15-22 bar) typically installed in the SCCI in the past. Export electricity generation from sugar-mills is dependent on the steam pressure of the boiler, as demonstrated by Venkatesh and Roy[67], whom reported that the installation of a 66 bar boiler allowed for an electricity export of 0.067 MW/WTC, while Moor 2008 reported an electrical export of 0.04MW/WTC when a 45 bar boiler was installed. Nsaful et al [70] reported that increasing the biomass boiler pressure from 30 bar boiler to 40, 63 or 82 bar boilers had increased the potential export electricity by 17.3, 35.9 and 40.1%, respectively. Thus, integrating biofuel production in existing biomass processing facilities should consider high pressure boilers, to maximise the co-generation of surplus electricity production from available bio-residues.

The Biomass Integrated Gasification and Combined Cycle (BIGCC) is a more advanced and efficient system for electricity production than the high pressure boiler combined with a steam turbine. Bridgewater et al[76] compared a BIGCC and a high pressure boiler system that operated at about 45bar for the generation of electricity from woody feedstock. That study showed that the boiler-steam-turbine system only attained an efficiency of 24% while the BIGCC system had an efficiency of about 40%, which is the typical upper limit for BIGCC efficiency[77]. That study[76] also showed however, that the boiler-steam-turbine system was more economically viable than the BIGCC due to the capital costs of the latter. Similarly, it was found [78] that the BIGCC system was less economically viable compared to a high pressure boiler-steam-turbine system for generating electricity, and also when integrated into sugar mills[79]. Moon et al[80] reported the contrary conclusion with regards to the economic comparison between gasification systems and combustor systems. The most likely explanation for this apparent discrepancy is the status of technological costs on the learning curve. Bridgewater et al[76] and others[78,79] based costs of the BIGCC system on emerging technological cost estimates, while the ordinary combustor system was based on mature costs. In Moon et al[80], the cost basis for the BIGCC was already maturing and was thus subject to some degree of cost reduction.

3 Industrial integration of biofuel

3.1 THE ECONOMIC POTENTIAL OF INDUSTRIAL INTEGRATION

Investigations that concern the integration of second generation biofuel production into the sugar cane crushing industry have focused primarily on the integration of lignocellulosic ethanol production into Autonomous Ethanol Distilleries [17,81,82], which forms part of the SCCI in Brazil. The studies by Dias et al[17,82] comprehensively showed that integrated first and second generation of ethanol from sugarcane is economically advantageous over separate first and second generation ethanol, as the IRRs obtained for the first, second generation and integrated scenarios where 14.9%,

10% and 16.8% respectively. In the analysis of Macrelli et al[81], the production costs of the individual first and second generation production costs, and their contribution to the integrated costs, were quantified, and the production cost of the second generation fuel was 0.77 US$/l for obtaining an IRR of 10%. Compared to the values in Table 1, it is higher than the costs obtained by Humbird et al[1], since the cost of enzyme used in the latter was the "on-site" production cost of 0.12 US$/l, while Macrelli et al[81] considered a purchased enzyme cost of 0.36 US$/l. Adjusting the cost of Macrelli et al[81] for the lower enzyme cost brings the production cost of integrated lignocellulosic ethanol to 0.53 US$/l, which met the selling price of the fossil equivalent. While this outcome is still not feasible for an investment needing a high IRR, this comparative analysis shows that integration of second generation biofuels into existing sugar mills (distilleries) can significantly reduce the production cost of second generation biofuels.

Previous studies that concerned the economic feasibility for integrating lignocellulosic fuels into the pulp and paper industry encompassed both bioethanol [83] and gasification-synthesis routes[59], primarily for Kraft processes. For the bioethanol route, Huang et al[83] considered the pre-extraction of hemicellulose fractions from chipped wood prior to digestion, in addition to the short cellulose fibres that was recovered from the Kraft process, for conversion to ethanol via fermentation. In order for the project to have met an interest rate of 10%, the MESP was determined at 0.65 US$/l, which was lower than the price of 0.75 US$/l that was reported for the standalone scenario in the USA. This price was still not competitive with the USA based fossil equivalent of 0.53 US$/l, probably due to the energy demands of the ethanol process. Integrating waste heats between the Kraft and ethanol processes with Pinch Point Analysis, could have lowered the energy costs of ethanol production and consequently, the MESP.

With regards to the integration of gasification-synthesis processes into the paper and pulp industry, Consonni et al[59] considered the gasification of black liquor and biomass residues to generate syngas that was to be used for the synthesis of FT syncrude. The IRR, based on the commercial price of the FT syncrude of 0.36 US$/l translated to an average price of gasoline and diesel at 0.75 US$/l, was calculated at 18%. Thus, integration also improved the investment potential of gasification-synthesis processes, when compared to the standalone process in Table 1, since the IRR achieved was significantly higher and it was based on fuel selling prices that was comparable to the fossil equivalents.

3.2 Benefits Associated with Integration

It has been shown that integration of second generation biofuels production into the P&PI and SCCI could yield more favourable economic outcomes than standalone second generation processes. One reason is that integration allows for the lignocellulosic biofuel process to benefit from the process units existing in the "host" process. In the case of integrated first-second generation from sugarcane[17,81,82], the ethanol streams derived from cane juice and bagasse share the same purification system and energy utilities (steam and electricity) generation system. The integration of ethanol into the Kraft Process[83] benefits from the energy generation equipment, which according to Humbird et al[1], bears 28% of the equipment cost of a standalone plant. For the example cited for the integrated gasification-synthesis fuel production[59] however, the FT fuel production process did not benefit from the Kraft Process in terms of sharing process/utility units in any appreciable manner. The black-liquor however, which is the primary fuel for gasification, was in a liquid state that had therefore eased the application of pressurised gasification systems[84]. As noted before, pressurised systems reduce downstream compression costs that are associated with atmospheric gasification systems.

The reduction of the cost of feedstock for lignocellulosic fuels that occurs with integration is another reason for the superior economic outcomes associated with integrated fuel production when compared to standalone second generation. Feedstock for stand-alone facilities are obtained by harvesting agricultural residues such as cornstover, or as low value crops such as switch grass, and the selling price of such residues in literature had ranged at 4.1-5.3 $/GJ[1,8]. For stand-alone biofuel facilities using sugarcane bagasse, it was considered that feedstock was sold from cane crushing operations at a coal equivalent price of 4.0 US$/GJ[10]. With biofuel integration into sugar mills, bagasse becomes available as feedstock to an integrated facility when the mill is upgraded to operate more efficiently. Thus, the cost associated with bagasse is the capital cost required to upgrade the energy efficiency of the mill. From literature[61,64], it is estimated that for a typical mill in South Africa operating at 300 wet tons of cane per hour, the capital cost required to improve the efficiency amounts to a normalised cost of bagasse of 0.3 US$/GJ. In the case of P&PI, where biofuels are produced from spent digestion liquor, the net energy needs could be fulfilled with low quality residues such as bark and hog-fuel. In the case of the Saiccor mill, where bark is land-filled, using bark for supplementing the energy needs negates the costs of land-filling. Else, the costs of hog-fuel for supplementing energy needs ranged at 1.5-1.8 US$/GJ in literature[85,86]. Thus, the costs associated with biomass feedstock for standalone facilities is at least twice the amount of the costs associated with residues used in integrated biofuel configurations.

According to Hamelinck and Faaij[87], the costs associated with the biomass feedstock contributes 45-58% of the operational costs of the stand-alone facility for 2G bioethanol production. In that study, it was estimated that the operational costs of ethanol production would reduce by 40% if the cost of feedstock was abated. Regarding gasification-synthesis process such as methanol and Fischer-Tropsch (FT) fuels synthesis, the operational costs would reduce by 43-48% if the feedstock costs are abated. A further complication with the logistics of “stand-alone” second generation plants is that economies of scale do not necessarily reduce the specific production costs, as larger

plants require that biomass is transported from further locations, which increases transportation costs[88]. Thus, improving economies of scale will only compensate for feedstock costs till certain scales, as Amigun et al[88] had demonstrated that the cost of methanol production reduced by 33% when increasing from thermal inputs of 100MW to 800MW, and only had a marginal decrease of <5% when the scale was increased to 2000MW.

4 Flow Sheet Analysis

Previous studies[6,8,89] have demonstrated the importance of process optimisation for second generation fuel production through flow sheet analysis, a technique primarily based on process simulations in Aspen Plus®[90] to which economic analysis are coupled. To arrive at the most economically viable process design for stand-alone FT fuels production for example, Tijmensen et al[6] developed various flow sheets, by combining alternative gasification designs with alternative FT reactor configurations. It was shown that pressurised gasification combined with advanced FT reactor technology was most viable, while atmospheric-air gasification combined with conventional FT reactor configurations are least viable, since conventional FT reactor technology and atmospheric-air gasification had excess capital and operational costs. A similar analysis for biomethanol production[55] had shown that regardless of the method of gasification and reactor technology, recycle streams are essential to improve the yield of liquid product, so the specific production costs can be reduced.

In the study [59] that determined the most viable option for integrating FT fuels production with a pulp mill, a scenario where a portion of the synthesis was diverted for heat and power generation against a scenario where all syngas went to the FT reactor was compared. It was shown that the scenario where syngas was diverted offered a slight advantage in investment potential since it exported more electricity, which was favoured in that particular economic context where the price

of electricity relative to the price of oil was 2.0 $.MJ^{-1} of electricity per $.MJ^{-1} of oil. In a South African context, this ratio of the electricity price to the oil price is 1.6 $.MJ^{-1} (based on prices from Eskom[91] and Department of Energy[92]), which shows that the same result might not be obtainable.

Flow-sheet analysis has also been used to demonstrate the effects of expected technological improvements on the overall performance of a biofuel process. In a study pertaining to bioethanol production by integrating the second generation bioethanol route into autonomous ethanol distilleries, Dias et al[17] developed processes based on the states of technology for hydrolysis and fermentation that are to be expected with 2010 and 2015 time frames. It was shown that yeasts capable of efficiently fermenting pentose sugars was the most significant factor in assuring low production costs. Those authors also showed a similar outcome in a separate study[82], although increasing process complexity by alkaline delignification in order to improve hydrolysis yields had resulted in unnecessary costs. Furthermore, those authors in a separate study[93] also showed that vacuum induced "multi-effect" distillation is advantageous over the conventional distillation in terms of utility consumption, especially when considering power generation techniques such as BIGCC, that have high electricity generating efficiencies. In another study pertaining to integrating second generation bioethanol processes into ethanol distilleries, Macrelli et al[81] demonstrated that heat integration to lower the process energy demands and integrating process streams for identical unit operations are important steps to lowering production costs. For stand-alone second generation ethanol production, quantifying the technological progress of the various steps in the bioethanol processes on the overall process performances were demonstrated by flow sheet analysis[94,95].

Flow sheet analysis has also been used to demonstrate the effect of Pinch Point Analysis (PPA) on the utility usage of biofuel processes, and hence, the overall efficiency. Dias et al[96]. had shown

that the application of PPA on first generation ethanol production had reduced the steam consumption by about 32%, while Petersen et al[4] had shown that the application of PPA on second generation biofuels improves the efficiency by about 5 percentage points. PPA is an algorithm that integrates the thermal energy of streams and units within a process in order to reduce the reliance on heating and cooling utilities[97,98]. For both the endothermic and exothermic energies, the magnitude and temperatures are qualified as respective cold and hot profiles called "composite curves" on a Cartesian plane, with the heat magnitude on the X-axis and temperature on the Y-axis. A heat magnitude is then calculated to shift the cold composite curve, so that the closest distance between the profiles (pinch region) corresponds to the minimum approach temperature. This magnitude then represents the cooling requirement, while the portion of the cold composite that is not overlapped by the hot composite curve above the pinch region is the heating requirement.

Thus, it is seen that flow sheet analysis had been used to assess the impact of process scenarios from various perspectives. In some studies, optimised flow sheet configurations have been found through assessing the outcomes of the various combinations of process unit alternatives in the various process stages[6,13,55,82]. Others have sought to determine the effect of the improvements that are to expected for individual process units on the entire process, thus providing a quantified motivation as to why research efforts should be focused on those improvements[17,94,95,99]. Furthermore, others have sought to determine the benefits that process intensification measures offers, such as heat integration and process stream combination[81].

5 Conclusions and limitations of Flow Sheet Technologies explorations in literature for integrated biofuel production

The literature relevant to the integrated production of bioethanol in the SCCI and P&PI has shown that, although integration significantly reduced the cost of production when compared to stand

alone second generation production, the cost of enzymes was still a significant concern [17,81,83,96]. Thus, even though integration had reduced biofuel production costs that were determined for the IRRs required for investments of low equity to debt ratios, it would not show promise in the context of high equity to debt to equity ratios, where IRRs are expected to reach the 25% value. Demonstrating the benefits associated with circumventing the costs of enzymes by only focusing on hemicellulose fermentation in integrated biofuel production from a perspective of process efficiency and economics through flow-sheet was not considered, though it had previously been suggested[100]. This mode of ethanol integration essentially builds on the concept of "value prior to combustion", which has been investigated as a stand-alone scenario by Treasure et al[86], where the hemicellulose that was extracted from grasses using autothermal hydrolysis was converted to ethanol, while the cellulose-lignin fractions was combusted, typically for electricity generation.

Though the production of bioethanol from hemicellulose in the form of SSL is an established industrial application, detailed flow sheet studies of these processes for identifying flow sheet configurations that are energy efficient and economically feasible are not presented in the open literature. Furthermore, the current industrial practices are based on SSL substrates derived from softwoods, which mostly contains hexose sugars. Therefore, a reference point for the industrial performance of bioethanol production based on SSL that have a dominance of pentose sugars does not exist. Thus, the impact of ethanol production from SSL on the energy balance on the overall facility (i.e. pulping + ethanol production) is not known. It is expected that the purification of ethanol from the SSL-fermentation broth would be a major energy cost, due to the diluteness of sugars in the substrate. If the energy demands for these processes are sourced from fossil fuels, then it is expected that the biofuel life-cycle would have a net accrual of greenhouse gas emissions, because processes that have much higher concentrations of ethanol (such as the corn-ethanol

process, with about 100g/l ethanol in the fermentation broth[101]) only have marginal greenhouse gas reductions when powered with fossil energy sources.

Concerning gasification-synthesis processes, detailed investigations for these integrating these modes of fuel production into the energy balances of biomass-based industries have been limited to the P&PI, in particular Kraft Process[59,83], with some recent developments in the sodium based Sulphite Processes[102]. Thus, it is not known for Sulphite Processes that have digestion processes based on magnesium oxide, because the Chemrec Gasification™ Process which is used to convert the spent digestion liquor to syngas while recovering the chemicals required for digestion has currently been developed for residues containing metals that produce ashes with low melting temperature. Detailed investigations for integrating gasification-synthesis processes into the representatives of the SSCI by converting the trash and bagasse to synthetic fuels and cogenerating heat and power to service the host facility are not known in literature.

As host industries, the SSCI and P&PI are industries that are energy intensive, and it had been shown that the use of residues that are normally used to satisfy the energy demands as feedstock for biofuels resulted in a requirement to import additional energy sources to service the net energy demand of the combined facility. In the SSCI, it had been shown that 50% of the post-harvest residues on the field was required as boiler fuel to satisfy the energy balance when bagasse was used for ethanol production in an integrated setup[17,82],and to create a large enough scale for economic viability. Bioethanol production integrated into the P&PI industries[83] from pre-extracted hemicelluloses that would usually have been in the digestion liquor for fuelling the recovery boiler, led to an increased reliance on supplementation of the system with hog-fuel. Regarding the integration of gasification-synthesis pathways that involved the gasification of the digestion residue, all available residues in addition to purchased hog-fuels were also gasified so that

the synthesis processes could release enough exothermic heat to power the mill[59]. Thus, the efficient generation of heat and power is an important aspect of the flow-sheeting analysis that explores the integration of biofuel production in these industries.

It has been shown that employing flow-sheet analysis methods was instrumental in arriving at the optimal flow sheets for second generation bioethanol and gasification-synthesis processes, as well as for integrated biofuel production in the SSCI or P&PI. The improvements in economic viabilities that are to be expected from the technological improvements, such as improved fermentation yields and synthetic fuel technology, have been demonstrated. The use of alternative processing technologies in various processing stages has been assessed, though not always in a methodical manner to establish the interactions between technological options in various processing in terms of efficiency, investment potential and sustainability. Otherwise, the effect for process intensification measures such as heat integration with pinch point analysis have been evaluated, but it's necessity in terms of maximising the potential to integrate a second generation process into a host industry has not been established. The use of statistical methods to optimise parameters for processes such as gasification had shown to be an essential step for obtaining the maximum efficiency at the prescribed process conditions. This approach however, could be extended for coupling flow sheets configurations to statistical models that also considers the impact of process parameters on the financial characteristics.

6 References

[1] Humbird D, Davis R, Tao L, Kinchin C, Hsu D, Aden A, et al. Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol. National Renewable Energy Laboratory 2011.

[2] Leibbrandt NH, Knoetze JH, Gorgens JF. Comparing biological and thermochemical processing of sugarcane bagasse : An energy balance perspective. Biomass Bioenerg. 2011;35:2117–26.

[3] Sendelius J. Steam Pretreatment Optimisation for Sugarcane Bagasse in Bioethanol Production. Master of Science, Lund University 2005.

[4] Petersen A, Melamu R, Görgens J., Knoetze, J.HCheng H. Comparison of Second-Generation Processes for the Conversion of Sugarcane Bagasse to Liquid Biofuels- Part A: Energy efficiency, Pinch Point Analysis and Life Cycle Analysis. Energy Conversion and Management 2015;91:292–301.

[5] Klein-Marcuschamer D, Oleskowicz-popiel P, Simmons BA, Blanch HW. The Challenge of Enzyme Cost in the Production of Lignocellulosic Biofuels. Biotechnology and Bioengineering 2012;xxx:1–5.

[6] Tijmensen MJ., Faaij AP., Hamelinck C., Van Hardeveld MRM. Exploration of the possibilities for production of Fischer Tropsch liquids and power via biomass gasification. Biomass Bioenerg. 2002;23:129–52.

[7] Kreutz TG, Larson ED, Liu G, Williams RH. Fischer-Tropsch Fuels from Coal and Biomass. 25th Annual International Pittsburgh Coal Conference 2008.

[8] Larson ED, Jin H, Celik FE. Large-scale gasification-based coproduction of fuels and electricity from switchgrass. Biofuels Bioproducts and Refining 2009;3:174–94.

[9] Leibbrandt NH, Aboyade AO, Knoetze JH, Görgens JF. Process efficiency of biofuel production via gasification and Fischer – Tropsch synthesis. Fuel 2013;109:484–92.

[10] Leibbrandt NH. Techno-Economics Study for Sugarcane Bagasse to Liquid Biofuels in South Africa: A Comparison between Biological and Thermochemical Process Routes. PhD Dissertation Department of Process Engineering. University of Stellenbosch, University of Stellenbosch 2010.

[11] Justice S. Private Financing of Renewable Energy – A guide for policy makers,. Unep 2009.

[12] Caula AS. Are European Bioenergy Targets Achievable ? An Evaluation Based on Thermoeconomic Indicators. Eindhoven University of Technology, 2011.

[13] Liu G, Larson ED, Williams RH, Kreutz TG, Guo X. Making Fischer-Tropsch Fuels and Electricity from Coal and Biomass: Performance and Cost Analysis. Energy and Fuels 2011;25:415–37.

[14] Kazi FK, Fortman JA, Anex RP, Hsu DD, Aden A, Dutta A, et al. Techno-economic comparison of process technologies for biochemical ethanol production from corn stover q. Fuel 2010;89:S20–S28.

[15] Laser M, College D. Comparative analysis of effi ciency , environmental impact , and process economics for mature biomass refi ning scenarios. Biofuels Bioproducts and Refining 2009;3:247–70.

[16] Haarlemmer G, Boissonnet G, Imbach J, Setiera P-A, Peduzzia E. Environmental Science Second generation BtL type biofuels – a production cost analysis. Energy and Environmental Science 2012;5:8445–56.

[17] Dias MOS, Junqueira TL, Cavalett O, Cunha MP, Jesus CDF, Rossell CEV, et al. Integrated versus stand-alone second generation ethanol production from sugarcane bagasse and trash. Bioresour. Technol. 2012;103:152–61.

[18] Canilha L, Santos VT., Rocha GJ., Almeida e Silva J., Giulietti M, Silva S., et al. A study on the pretreatment of a sugarcane bagasse sample with dilute sulfuric acid. Journal of Industrial Microbiology and Biotechnology 2011.

[19] Aguilar R, Ramırez J., Garrote G, Vazquez M. Kinetic study of the acid hydrolysis of sugar cane bagasse. Journal of Food Engineering 2002;55:309–18.

[20] Jeevan P, Nelson R, Rena AE. Optimization studies on acid hydrolysis of Corn cob hemicellulosic hydrolysate for Microbial production of xylitol 2011;1:114–23.

[21] Paiva JED, Maldonade IR, Scamparini ARP. Xylose production from sugarcane bagasse by surface response methodology Produção de xilose a partir do bagaço de cana-de-açúcar por metodologia de superfície de resposta. Revista Brasileira De Engenharia Agrícola e Ambiental 2009;55:75–80.

[22] Martin C, Galbe M, Nilvebrant N, Jonsson L. Comparison of the Fermentability of Enzymatic Hydrolyzates of Sugarcane Bagasse Pretreated by Steam Explosion. Applied and Environmental Microbiology 2002;98-100:699–716.

[23] Rocha GJM, Martín C, Vinícius FN, Gómez EO, Gonçalves AR. Mass balance of pilot-scale pretreatment of sugarcane bagasse by steam explosion followed by alkaline delignification. Bioresour. Technol. 2012;111:447–52.

[24] Gírio FM, Fonseca C, Carvalheiro F, Duarte LC, Marques S, Bogel-Lukasik R. Hemicelluloses for fuel ethanol : A review. Bioresour. Technol. 2010;101:4775–800.

[25] Kurian J., Minu A., Banerji A, Kishore VV. Bioconversion of hemicellulose hydrolysate of sweet sorghum bagasse to ethanol by using Pichia Stipitis NCIM 3497 and Debaryomyces Hansenii SP. Bioresources 2010;5:2404–16.

[26] Nigam JN. Ethanol production from wheat straw hemicellulose hydrolysate by Pichia stipitis. Journal of Biotechnology 2001;87:17–27.

[27] Rudolf A, Baudel H, Zacchi G. Simultaneous Saccharification and Fermentation of Steam-Pretreated Bagasse Using Saccharomyces cerevisiae TMB3400 and Pichia stipitis CBS6054. Biotechnology and Bioengineering 2008;99:783–90.

[28] Mcmillan JDJ. Progress on Advanced Liquid Biofuels in the USA Biofuels. International Symposium on Alchohol Fuels, 2013.

[29] Bjorling T, Lindman B. Evaluation of xylose-fermenting yeasts for ethanol production from spent sulfite liquor. Enzyme Microbial Technology 1989;11:240–6.

[30] Nigam JN. Ethanol production from hardwood spent sulfite liquor using an adapted strain of Pichia stipitis. Journal of Biotechnology 2001;26:145–50.

[31] Helle SS, Murray A, Lam J, Cameron DR, Duff SJB. Xylose fermentation by genetically modified Saccharomyces cerevisiae 259ST in spent sulfite liquor. Bioresour. Technol. 2004;92:163–71.

[32] Bajwa PK, Shireen T, Aoust D, Pinel D, Martin VJJ, Trevors JT, et al. Mutants of the Pentose-Fermenting Yeast Pichia stipitis With Improved Tolerance to Inhibitors in Hardwood Spent Sulfite Liquor. Biotechnology and Bioengineering 2009;104:892–900.

[33] Helle SS, Lin T, Duff SJB. Optimization of spent sulfite liquor fermentation. Enzyme and Microbial Technology 2008;42:259–64.

[34] Rodsrud G. Biorefining - expanding the sulfite pulping biorefinery concept 2011.

[35] Magdzinski L. Tembec Temiscaming Integrated Biorefinery. Pulp & Paper Canada 2006;107:147–9.

[36] Mahishi MR, Goswami DY. Thermodynamic optimization of biomass gasifier for hydrogen production. International Journal of Hydrogen Energy 2007;32:3831–40.

[37] Prins M, Ptasinski K, Janssen F. From coal to biomass gasification : Comparison of thermodynamic efficiency. Energy 2007;32:1248–59.

[38] Filippis PD, Borgianni C, Paolucci M, Pochetti F. Gasification process of Cuban bagasse in a two-stage reactor. Biomass Bioenerg. 2004;27:247–52.

[39] Puig-arnavat M, Bruno JC, Coronas A. Review and analysis of biomass gasification models. Renew. Sustain. Energ. Rev. 2010;14:2841–51.

[40] Schuster G, L o,er G, Weigl K, Hofbauer H. Biomass steam gasi ® cation ± an extensive parametric modeling study. Bioresour. Technol. 2001;77:71–9.

[41] Holmgren KM, Berntsson T, Andersson E, Rydberg T. System aspects of biomass gasification with methanol synthesis e Process concepts and energy analysis. Energy 2012;45:817–28.

[42] Craig KR, Mann MK. Cost and Performance Analysis of Biomass-Based Integrated Gasification Combined-Cycle (BIGCC) Power Systems Cost and Performance Analysis of Biomass-Based Integrated Gasification Combined-Cycle (BIGCC) Power Systems. National Renewable Energy Laboratory 1996.

[43] Abdelouahed L, Authier O, Mauviel G, Corriou JP, Verdier G, Dufour A. Detailed Modeling of Biomass Gasification in Dual Fluidized Bed Reactors under Aspen Plus. Energy and Fuels 2012;26:3840−3855.

[44] Baratieri M, Baggio P, Fiori L, Grigiante M. Biomass as an energy source : Thermodynamic constraints on the performance of the conversion process. Bioresour. Technol. 2008;99:7063–73.

[45] Dupont C, Boissonnet G, Seiler J-marie, Gauthier P, Schweich D. Study about the kinetic processes of biomass steam gasification. Fuel 2007;86:32–40.

[46] Rapagna S, Jand N, Foscolo PU. Catalytic gasification of biomass to produce hydrogen rich gas. Int. J. Hydrog. Energ. 1998;23:551–7.

[47] He M, Xiao B, Liu S, Guo X, Luo S, Xu Z, et al. Hydrogen-rich gas from catalytic steam gasification of municipal solid waste (MSW): Influence of steam to MSW ratios and weight hourly space velocity on gas production and composition. Int. J. Hydrog. Energ. 2009:1–10.

[48] Silva V, Rouboa A. Optimizing the gasification operating conditions of forest residues by coupling a two-stage equilibrium model with a response surface methodology. Fuel Process. Technol. 2014;122:163–9.

[49] M Van Der Meijden C, Veringa HJ, Rabou LPLM. The production of synthetic natural gas (SNG): A comparison of three wood gasification systems for energy balance and overall efficiency. Biomass Bioenerg. 2010;34:302–11.

[50] Sun L, Smith R. Rectisol wash process simulation and analysis. J. Clean. Prod. 2013;39:321–8.

[51] Zainal ZA, Ali R, Lean CH, Seetharamu KN. Prediction of performance of a downdraft gasi ® er using equilibrium modeling for di erent biomass materials. Energy Conversion and Management 2001;42:1499–515.

[52] Ryan L, Campbell N. Spreading the net: The multiple benefits of energy efficiency improvements. 2012.

[53] Brown MA. Market failures and barriers as a basis for clean energy policies $. Energ. Policy 2008;29:1197–207.

[54] Phillips SD, Tarud JK, Biddy MJ, Phillips SD, Tarud JK, Biddy MJ. Gasoline from Wood via Integrated Gasification, Synthesis, and Methanol-to- Gasoline Technologies. 2011.

[55] Hamelinck CN, Faaij AP. Future prospects for production of methanol and hydrogen from biomass. 2001.

[56] Tijm PJA, Waller FJ, Brown DM. Methanol technology developments for the new millennium. Applied Catalysis A: General 2001;221:275–82.

[57] Dry ME. The Fischer – Tropsch process : 1950 – 2000. Catalyst Today 2002;71:227–41.

[58] Ekbom T, Hjerpe C, Hermann F. Pilot study of Bio-jet A-1 fuel production for Stockholm-Arlanda Airport. Stockholm: 2009.

[59] Consonni S, Katofsky RE, Larson ED. Chemical Engineering Research and Design A gasification-based biorefinery for the pulp and paper industry. Chem. Eng. Res. Des. 2009;7:1293–317.

[60] Ensinas AV, Nebra SA, Lozano MA, Serra LM. Analysis of process steam demand reduction and electricity generation in sugar and ethanol production from sugarcane. Energy Conversion and Management 2007;48:2978–87.

[61] Peacock S. Process Design for Optimum Energy Efficiency. Tongaat Hullet Sugar 2008.

[62] VAN DER WESTHUIZEN WA. A TECHNO-ECONOMIC EVALUATION OF INTEGRATING FIRST AND SECOND GENERATION BIOETHANOL PRODUCTION FROM SUGARCANE IN SUB-SAHARAN AFRICA. Stellenbosch University, 2012.

[63] Nsaful F. PROCESS MODELLING OF SUGAR MILL BIOMASS TO ENERGY CONVERSION PROCESSES AND ENERGY INTEGRATION OF PYROLYSIS. Stellenbosch University, 2012.

[64] Wienese A, Purchase BS. RENEWABLE ENERGY : AN OPPORTUNITY FOR THE SOUTH AFRICAN SUGAR INDUSTRY ? Proceedings: The SouthAfrican Sugar Technologists' Association, vol. 78, n.d.

[65] Ogden J., Hochgreb S, Hylton M. Steam economy and cogeneration in cane factories. International Sugar Journal 1990;92.

[66] Botha T, Von Blottnitz H. A comparison of the environmental benefits of bagasse-derived electricity and fuel ethanol on a life-cycle basis. Energ. Policy 2006;34:2654–61.

[67] Venkatesh KS, Roy AS. Development and Installation of High Pressure Boilers for Co-Generation Plant in Sugar Industries. Smart Grid and Renewable Energy 2010;1:51–3.

[68] Mbohwa C, Fukuda S. Electricity from bagasse in Zimbabwe. Biomass Bioenerg. 2003;25:197–207.

[69] Seabra JEA, Tao L, Chum HL, Macedo IC. A techno-economic evaluation of the effects of centralized cellulosic ethanol and co-products refinery options with sugarcane mill clustering. Biomass Bioenerg. 2010;34:1065–78.

[70] Nsaful F, Görgens JF, Knoetze JH. Comparison of combustion and pyrolysis for energy generation in a sugarcane mill. Energy Conversion and Management 2013;74:524–34.

[71] U.S. Environmental Protection Agency. Available and Emerging Technologies for Reducing Greenhouse Gas Emissions from the Pulp and Paper Manufacturing Industry. North Carolina: 2010.

[72] Sappi Group. Saiccor Presentation 2011.

[73] Marques AP, Evtuguin DV, Magina S, Amado L, Prates A. Composition of Spent Liquors from Acidic Magnesium – Based Sulphite Pulping of Eucalyptus globulus. Journal of Wood Chemistry and Technology 2009:37–41.

[74] Martin N, Anglani N, Einstein D, Khrushch M, Worrell E, Price LK. Opportunities to Improve Energy Efficiency and Reduce Greenhouse Gas Emissions in the U . S . Pulp and Paper Industry. 2000.

[75] Moor B. MODERN SUGAR EQUIPMENT ASSISTING COGENERATION. 2008.

[76] Bridgwater AV, Toft AJ, Brammer JG. A techno-economic comparison of power production by biomass fast pyrolysis with gasification and combustion. Renew. Sustain. Energ. Rev. 2002;6:181–248.

[77] Wang L, Weller CL, Jones DD, Hanna MA. Contemporary issues in thermal gasification of biomass and its application to electricity and fuel production. Biomass Bioenerg. 2008;32:573–81.

[78] Caputo AC, Palumbo M, Ã PMP, Scacchia F. Economics of biomass energy utilization in combustion and gasification plants : effects of logistic variables. Biomass Bioenerg. 2005;28:35–51.

[79] Ramjatun S, Gukhool J, Seebaluck D. OPTIMISATION OF POWER GENERATION. Science and Technology 1999;3:79–86.

[80] Moon J-hong, Lee J-woo, Lee U-do. Economic analysis of biomass power generation schemes under renewable energy initiative with Renewable Portfolio Standards (RPS) in Korea. Bioresour. Technol. 2011;102:9550–7.

[81] Macrelli S, Mogensen J, Zacchi G. Techno-economic evaluation of 2 nd generation bioethanol production from sugar cane bagasse and leaves integrated with the sugar-based ethanol process. Biotechnol. Biofuel. 2012;5:22.

[82] Dias MOS, Cunha MP, Jesus CDF, Rocha GJM, Geraldo J, Pradella C, et al. Second generation ethanol in Brazil : Can it compete with electricity production ? Bioresour. Technol. 2011;102:8964–71.

[83] Huang H-jiang, Ramaswamy S, Al-dajani WW, Tschirner U. Process modeling and analysis of pulp mill-based integrated biorefinery with hemicellulose pre-extraction for ethanol production : A comparative study. Bioresour. Technol. 2010;101:624–31.

[84] Dahmen N, Henrich E, Dinjus E, Weirich F. The bioliq® bioslurry gasification process for the production of biosynfuels, organic chemicals, and energy. Energy, Sustainability and Society 2012;2:1–44.

[85] Anderson N, Chung W, Loeffler D, Jones JG. A Productivity and Cost Comparison of Two Systems for Producing Biomass Fuel from Roadside Forest Treatment Residues. Forest Products Journal 2012;62:222–33.

[86] Treasure T, Gonzalez R, Venditti R, Pu Y, Jameel H, Kelley S, et al. Co-production of electricity and ethanol , process economics of value prior combustion. Energy Conversion and Management 2012;62:141–53.

[87] Hamelinck C., Faaij AP. Outlook for advanced biofuels. Energ. Policy 2006;34:3268–83.

[88] Amigun B, Gorgens J, Knoetze H. Biomethanol production from gasification of non-woody plant in South Africa : Optimum scale and economic performance. Energ. Policy 2010;38:312–22.

[89] Hamelinck CN, Hooijdonk GV, Faaij AP. Ethanol from lignocellulosic biomass: techno-economic performance in short-, middle- and long-term. Biomass Bioenerg. 2005;28:384–410.

[90] Aspen Technology Inc. Aspen Plus®, Aspen Icarus® 2008.

[91] Eskom Tariffs and Charges (www.eskom.co.za/content)

[92] Department of Energy (www.energy.gov.za)

[93] Dias MOS, Ensinas AV, Nebra SA, Filho R., Rossell CEV, Regina M, et al. Production of bioethanol and other bio-based materials from sugarcane bagasse : Integration to conventional bioethanol production process. Chem. Eng. Res. Des. 2009;7:1206–16.

[94] Humbird D, Aden A. Biochemical Production of Ethanol from Corn Stover : 2008 State of Technology Model Biochemical Production of Ethanol from Corn Stover : 2008 State of Technology Model. National Renewable Energy Laboratory 2009.

[95] Aden A. Biochemical Production of Ethanol from Corn Stover 2007 State of Technology Model Technical Report. National Renewable Energy Laboratory, Harris Group. 2007.

[96] Dias MOS, Modesto M, Ensinas AV, Nebra SA, Maciel R, Rossell CEV. Improving bioethanol production from sugarcane : evaluation of distillation , thermal integration and cogeneration systems. Energy 2011;36:3691–703.

[97] Kemp I. Pinch Analysis and Process Integration: A User Guide on Process Integration for the Efficient Use of Energy, Second Edition. Elsevier 2007.

[98] March L. Introduction to Pinch. Linnhoff March LTD; 1998.

[99] Hamelinck C., Hooijdonk GV, Faaij AP. Ethanol from lignocellulosic biomass : techno-economic performance in short- , middle- and long-term. Biomass Bioenerg. 2005;28:384–410.

[100] Purchase BBS, Walford SN, Waugh EJ. AN UPDATE ON PROGRESS IN THE PRODUCTION OF ETHANOL FROM BAGASSE. Proceedings a/The SouthAfrican Sugar Technologists' Association - June 1986 1986:33–6.

[101] Mcaloon A, Taylor F, Yee W, Regional E, Ibsen K, Wooley R, et al. Determining the Cost of Producing Ethanol from Corn Starch and Lignocellulosic Feedstocks Determining the Cost of Producing Ethanol from Corn Starch and Lignocellulosic. National Renewable Energy Laboratory 2000.

[102] Landalv I, Furusjo E, Stare R. Patent WO2011123034A1 - Gasification of sulphite thick liquor - Google Patents. WO2011123034 A1, 2013.

.

Chapter 3: Overall Work-plan, Hypothesis and Dissertation Structure

1 Overall Work-plan

The overall aims of this project were to develop cost effective processes for second generation biofuel production in South Africa, through integration into the Sugar Cane Crushing and Pulp & Paper Industries (i.e. SSCI and P&PI). In South Africa, the SSCI is represented by the RSI and the PPI by Sulphite Processes. This would be achieved by simulation of industrial processes, flow sheet analysis, economic assessment and determination of environmental impacts. The work-plan, which basically amounted to flow-sheet development, was designed to encompass the technical aspects to ensure a self-sustaining process; economic aspects to ensure that the production of biofuels is viable from an investment point of view; and environmental aspects to ensure that the anticipated environmental benefits of second generation biofuels are maintained. These objectives were designed to address shortcomings identified in scientific literature on the topic of integration of second generation biofuels production into these industrial facilities.

1.1 General Methodology and Envisagement

The underlying methodology to be employed in the flow-sheet analysis is process simulation in Aspen Plus®[1], based on experimental data and design elements found in verified literature. The results will be used to characterise the technical performances indicators, such as fuel output, electricity output, utility demands and availability. Results from the process simulations will be used to determine the capital investment costs and key economic indicators (KEI), such as the Internal Rate of Return (IRR) and minimum fuel selling price (MFSP), both of which are measures of the attractiveness of biofuels production from an investment (returns on invested capital) perspective. Economic modelling will be carried out with Risk Based Economic Assessments, which are based on

Monte Carlo Methods in order to establish the risk associated with the KEIs [2–4] and there viabilities to private investors. Where processes involve a significant use of energy from fossil sources, results from process simulation will be used to calculate the greenhouse gas reductions associated with the life cycle of the fuel product, using documented methods[5,6] with supporting databases and software (GREET[7] and SimaPro[8]). Improvements to flow-sheets are incorporated into the simulations, to ensure that the desired environmental benefits of second generation biofuels production are preserved.

In this dissertation, it is envisaged that flow-sheet analysis be used to establish the relationship between technological processing options used in various processing stages, in terms of the energy-efficiency and economic characteristics of the flow-sheet. Furthermore, the necessity of process intensification measures such as Pinch Point heat integration[9–11] in the context of integrating biofuel production into an energy intensive industrial process will be determined. It is also planned to combine flow-sheet analysis with statistical methods to arrive at process conditions that are optimised economically and technically, and also subjected to the constraints that the process imposes. Thus, from such analysis, deductions can be made on the cause of viability (or un-viability) of individual process technologies and/or the combinations there-of.

1.2 SECOND GENERATION BIOFUEL INTEGRATED INTO THE RAW SUGAR MILLS

Integration of second generation biofuels into existing sugar mills (i.e. the RSI) in South Africa will require modernisation of the processing equipment and unit operations with more energy efficient technologies, so that steam demands of the mill are reduced to 0.40 tons of steam per ton of cane processed [12]. The capital costs of such modernisation should therefore be reflected in the costs of integrating second generation biofuels or advanced electricity generation into a sugar mill. Furthermore, the older sugar mills in South Africa have traditionally used low pressure boilers that

are inefficient at steam and electricity generation, and thus modernisation for the purpose of exporting bio-energetic products should include the replacement of the existing low pressure boiler with higher pressure boilers[12–14]. The combination of the biofuel production process with the new boilers and gas/steam turbines for electricity generation, would therefore supply all of the process energy requirements (steam, electricity) of the modernised sugarcane mill[15,16]. Optimisation of energy efficiency in sugarcane processing will maximise the conversion of lignocellulose to biofuels, while energy optimisation of the combined sugar-mill and energy production processes will maximise the amounts of biofuels and/or surplus electricity for export to the grid, produced from these integrated facilities. Thus, several aspects of flow-sheet development and technology selection have to be addressed in the development of integrated scenarios, with co-production of biofuels and/or electricity by modernised, existing sugar mills.

Integration of second generation bio-ethanol production into sugar-mills will explore an alternative to the traditional conversion of the cellulose components to bioethanol, which includes the costly process of enzymatic hydrolysis[16,17]. Instead, process flow-sheets for the conversion of only the hemicellulose sugars[18] that are obtained through conventional pre-treatment's will be investigated. This avoids the need for enzymatic hydrolysis of cellulose, while also providing a combustible cellu-lignin residue fuel that is suitable for co-generation of electricity from sugarcane lignocelluloses. Flow-sheet and technological options for a combined process, producing both bio-ethanol and surplus electricity for export to the grid, will thus be investigated. The economic attractiveness of such a combined process would have to show an improvement compared to a process where the entire lignocellulose feedstock is converted to electricity, which is the conventional approach for electricity co-generation in sugar mills[16,17]. As various process technologies and process intensification measures are available for the combined ethanol-electricity process, systematic flow-sheet analysis of possible technology-combinations is required, to identify preferred and robust process options that fulfil the requirements of economic and environmental

viability, as described in Chapter 4. Heat integration by Pinch Point Analysis is a key method in process intensification and ensuring that high conversion/energy efficiencies are achieved in the process integration scenarios.

An alternative method of second generation biofuels production in the sugar industry is the conversion of lignocellulose to methanol or FT syncrude, through gasification-synthesis technologies. Gasification-synthesis processes will therefore be compared to fermentation-based processes, in terms of energy yields, economics and environmental impacts, as described in Chapter 6. Given that the amount of bagasse and trash available for processing equates to 0.2 tons per ton of sugarcane processed[16,19], then an integrated FT synthesis plant could hypothetically provide the steam requirements of a modern sugarcane mill that is expected to operate with a steam demand of 0.4 tons of steam per ton of cane, since the total steam produced would equate to about 0.6 tons per ton of cane. A steam balance for methanol synthesis however, shows that the exhaust steam available from the turbines is about 0.7 ton per ton of biomass processed[20], without considering the waste heats that was dispensed to the environment. Thus, it would have to be ascertained whether integrating methanol synthesis into a sugar mill is capable of servicing the process energy requirements of the sugar-mill, which is an essential requirement for integrated production of biofuels. This will be addressed through adequate heat integration between the sugar mill and waste heats of the methanol synthesis process. Furthermore, as the major costs of a gasification-synthesis process lies in the production of clean, compressed syngas, it is envisaged that the sub-process for producing the conditioned syngas be optimised to meet the requirements for synthesis processes in an efficient and costs effective manner, as part of technology selection options to be investigated.

1.3 SECOND GENERATION BIOFUEL INTEGRATED INTO THE P&PI

In this dissertation, focus on the potential of SSL from an MgO-based sulphite pulping process as a feedstock for second generation bio-ethanol production will be explored, as this SSL contains mostly pentose sugars originating from hardwood-pulping that is implemented on a large-scale in South Africa. The conversion of pentose sugars in SSL to ethanol by robust strains has been efficiently done at high concentrations of dissolved solids (20-30%) on a laboratory scale[21]. However, the conversion of SSL to ethanol as an export product, will result in a deficit in the energy-balance of the sulphite pulping process, as SSL is presently burnt to provide some of the required process steam [22,23]. Flow-sheet analysis for ethanol production from SSL would thus also explore alternative sources of renewable fuel, to fulfil the process energy requirements of the sulphite mill. As an example, the Saiccor sulphite pulping process presently augments the supply of process energy from biomass sources with the combustion of coal, which is associated with significant greenhouse gas emissions. The deficit in process energy supply, caused by ethanol production from SSL, would thus be resolved either by (i) increasing the reliance of coal or (ii) installation of a bark boiler to take advantage of the bark that is currently disposed in a landfill, and/or (iii) incorporation of a biodigester to produce biogas as supplementary fuel from the organics in the liquid effluents that could supplement the recovery boiler. Flow-sheeting, economic and environmental assessment would identify the most appropriate process solutions for integration of ethanol production from SSL into a sulphite mill, such as the Saiccor facility, as described in Chapter 5.

The combustion of MgO-based SSL is presently done to both recover process energy and pulping chemicals. A possible alternative is the gasification of SSL, but gasification technology for MgO-based SSL has not shown to be technically viable yet, and thus, gasification at MgO-based Sulphite Mills would only focus on bark residues. Such a gasification process can be considered both for the provision of process energy requirements of the sulphite pulping process, and provision of syngas for

production of synthetic fuels. An expansion to the integrated facility, producing ethanol from SSL, with a gasification-synthesis process for bark will thus be investigated through flow-sheet development and economic/environmental assessments. Such a facility would thus produce two biofuels (ethanol and synthetic fuel) using the residues from the existing pulping process, as described in Chapter 7.

2 Hypothesis

It is hypothesised that through the course of this dissertation, viable integrated biofuel production process in the RSI and P&PI are going to be achieved, as the work-plan envisaged encompasses a range of technical, cost and environmental effective techniques in flow-sheet developments.

3 Dissertation Structure and Workflow

The structure and workflow of the dissertation is graphically depicted in Figure 5.

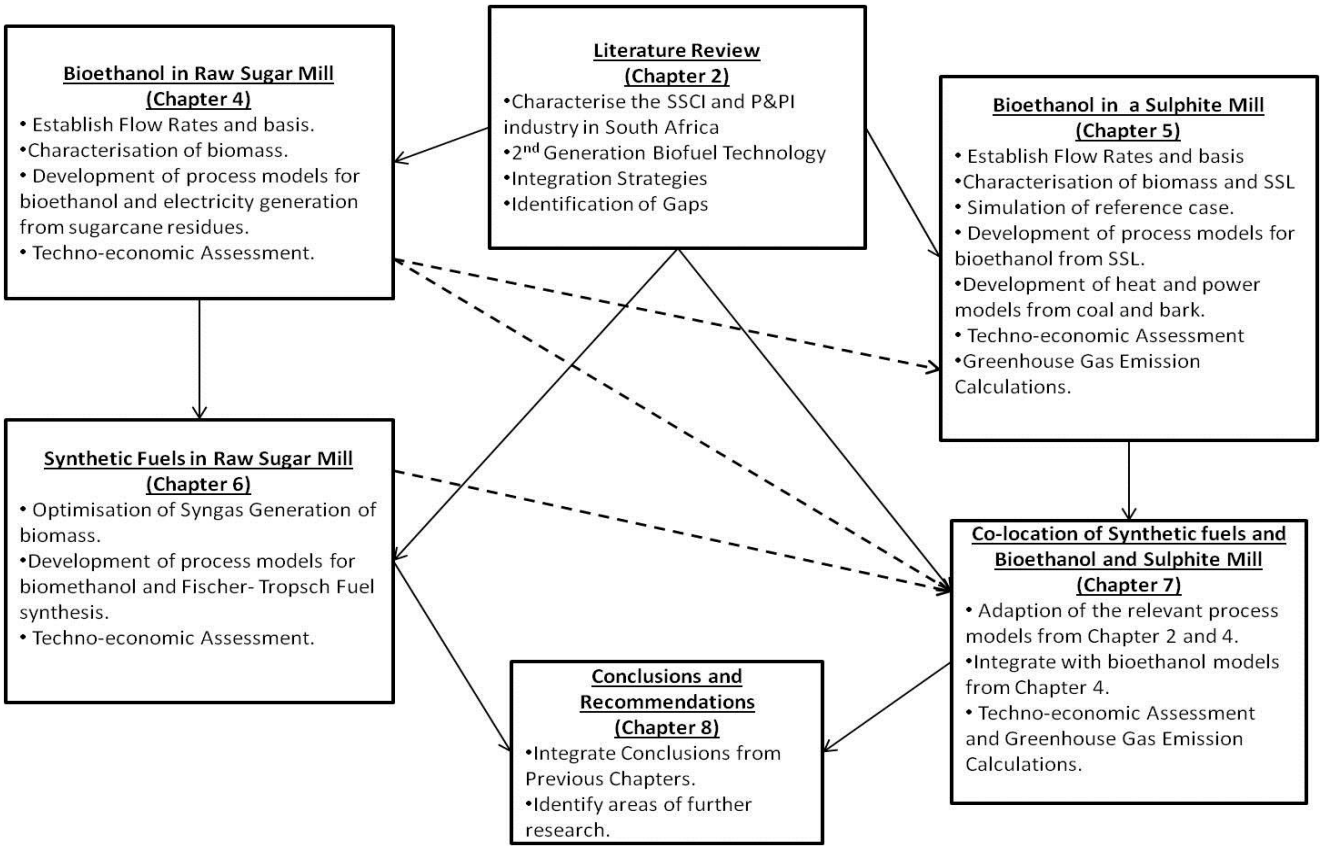


Figure 5: Detailed Workflow and Structure of Dissertation

4 References

[1] Aspen Technology Inc. Aspen Plus®, Aspen Icarus® 2008.

[2] Richardson JW, Herbst BK, Outlaw JL, Anderson DP, Klose SL, Gill II RC. Risk Assessment in Economic Feasibility Analysis: The Case of Ethanol Production in Texas. 2006.

[3] Richardson JW, Lemmer WJ, Outlaw JL. Bio-ethanol Production from Wheat in the Winter Rainfall Region of South Africa : A Quantitative Risk Analysis. Int. Food. Argibus. Manag. Rev. 2007;10:181–204.

[4] Amigun B, Petrie D, Görgens J. Economic risk assessment of advanced process technologies for bioethanol production in South Africa : Monte Carlo analysis. Renewable Energy 2011;36:3178–86.

[5] Ecoivent. Life Cycle Inventories for Bioenergy. 2007.

[6] Hedemann J, König U, Cuche A, Egli N. Technical Documentation of the ecoinvent Database. vol. 01. 2003.

[7] Wang M, Burnham A, Wu Y. GREET 2007.

[8] PRé-Consultants. SimaPro 2010.

[9] Kemp I. Pinch Analysis and Process Integration: A User Guide on Process Integration for the Efficient Use of Energy, Second Edition. Elsevier 2007.

[10] March L. Introduction to Pinch. Linnhoff March LTD; 1998.

[11] IChemE. Pinch Point Analysis Spreadsheet 2006.

[12] Wienese A, Purchase BS. RENEWABLE ENERGY : AN OPPORTUNITY FOR THE SOUTH AFRICAN SUGAR INDUSTRY ? Proceedings: The SouthAfrican Sugar Technologists' Association, vol. 78, n.d.

[13] Venkatesh KS, Roy AS. Development and Installation of High Pressure Boilers for Co-Generation Plant in Sugar Industries. Smart Grid and Renewable Energy 2010;1:51–3.

[14] Moor B. MODERN SUGAR EQUIPMENT ASSISTING COGENERATION. 2008.

[15] Dias MOS, Cunha MP, Jesus CDF, Rocha GJM, Geraldo J, Pradella C, et al. Second generation ethanol in Brazil : Can it compete with electricity production ? Bioresour. Technol. 2011;102:8964–71.

[16] Macrelli S, Mogensen J, Zacchi G. Techno-economic evaluation of 2 nd generation bioethanol production from sugar cane bagasse and leaves integrated with the sugar-based ethanol process. Biotechnol. Biofuel. 2012;5:22.

[17] Dias MOS, Modesto M, Ensinas AV, Nebra SA, Maciel R, Rossell CEV. Improving bioethanol production from sugarcane : evaluation of distillation , thermal integration and cogeneration systems. Energy 2011;36:3691–703.

[18] Purchase BBS, Walford SN, Waugh EJ. AN UPDATE ON PROGRESS IN THE PRODUCTION OF ETHANOL FROM BAGASSE. Proceedings a/The SouthAfrican Sugar Technologists' Association - June 1986 1986:33–6.

[19] Dias MOS, Junqueira TL, Cavalett O, Cunha MP, Jesus CDF, Rossell CEV, et al. Integrated versus stand-alone second generation ethanol production from sugarcane bagasse and trash. Bioresour. Technol. 2012;103:152–61.

[20] Phillips SD, Tarud JK, Biddy MJ, Phillips SD, Tarud JK, Biddy MJ. Gasoline from Wood via Integrated Gasification, Synthesis, and Methanol-to- Gasoline Technologies. 2011.

[21] Helle SS, Murray A, Lam J, Cameron DR, Duff SJB. Xylose fermentation by genetically modified Saccharomyces cerevisiae 259ST in spent sulfite liquor. Bioresour. Technol. 2004;92:163–71.

[22] Huang H-jiang, Ramaswamy S, Al-dajani WW, Tschirner U. Process modeling and analysis of pulp mill-based integrated biorefinery with hemicellulose pre-extraction for ethanol production : A comparative study. Bioresour. Technol. 2010;101:624–31.

[23] Consonni S, Katofsky RE, Larson ED. Chemical Engineering Research and Design A gasification-based biorefinery for the pulp and paper industry. Chem. Eng. Res. Des. 2009;7:1293–317.

Chapter 4: Integration of Bioethanol Production in a Raw Sugar Mill

This has been published in the journal "Biotechnology for Biofuels", volume 7, Issue 105 and can be downloaded at http://www.biotechnologyforbiofuels.com/content/7/1/105. It has been reproduced in this dissertation with the permission of the BioMed publication house, with some minor textual improvements.

Title of Article: "Techno-economic comparison of ethanol and electricity coproduction schemes from sugarcane residues at existing sugar mills in Southern Africa"

Contribution to overall study

In this paper, flow sheet analysis was used to develop integrated processes for ethanol co-production and heat and power co-generation from sugarcane residues at sugar mills. These processes were compared to the exclusive co-generation of heat and power from the same residues, in terms of the technical and economic performances. In all process scenarios sugar mill modernisation is included in the capital expenditure, allowing co-generation of surplus electricity for export to the grid.

In relation to the overall objectives of this dissertation, it was observed that bioethanol production scenarios that are technically and economically feasible are possible when integrated into sugar mills. Such process scenarios were economically competitive against the exclusive generation of electricity. In relation to the general objectives of the dissertation, flow-sheet analysis was used to determine synergies between technologies in various processing stages, such as how

multi-effect distillation in ethanol purification is synergetic with Biomass Integrated Gasification with Combined Cycles in heat and power production. Furthermore, the necessity of pinch point analysis was established, as processes were either poorly efficient or incompatible for integration without it.

Author Contributions

AMP was the primary investigator into the work. He performed all simulations of the various processes and economic evaluations. He also completed the interpretation of results and was the primary author of the written text. MCA was the internal reviser who checked the paper critically for inconsistencies in the text and structure. He also gave assistance in the structuring of the paper. JFG is the study leader of the research group, reviewed the paper internally and approved the submission from our department. He is also the corresponding author. All authors agree to be accountable for all aspects of the work and will ensure that questions relating to accuracy and integrity be appropriately investigated and resolved. All authors read and approved the final manuscript.

Techno-economic comparison of ethanol and electricity coproduction schemes from sugarcane residues at existing sugar mills in Southern Africa

Abdul M Petersen[1] (AMP)

Email: abdulpetersen@gmail.com

Mathew C Aneke[1] (MCA)

Email: mathew.aneke@gmail.com

Johann F Görgens[1*] (JFG)

[*]Corresponding author

Email: jgorgens@sun.ac.za

[1]Department of Process Engineering, University of Stellenbosch, Cnr Banghoek Road & Joubert Street Stellenbosch, 7600, South Africa

Abstract

Background

The economics of producing only electricity from residues, which comprise of surplus bagasse and 50% post-harvest residues, at an existing sugar mill in South Africa was compared to the coproduction of ethanol from the hemicelluloses and electricity from the

remaining solid fractions. Six different energy schemes were evaluated. They include: (1) exclusive electricity generation by combustion with high pressure steam cycles (CHPSC-EE), (2) biomass integrated gasification with combined cycles (BIGCC-EE), (3) coproduction of ethanol (using conventional distillation (CD)) and electricity (using BIGCC), (4) coproduction of ethanol (using CD) and electricity (using CHPSC), (5) coproduction of ethanol (using vacuum distillation (VD)) and electricity (using BIGCC), and (6) coproduction of ethanol (using VD) and electricity (using CHPSC). The pricing strategies in the economic analysis considered an upper and lower premium for electricity, on the standard price of the South African Energy Provider Eskom' of 31 and 103% respectively and ethanol prices were projected from two sets of historical prices.

Results

From an energy balance perspective, ethanol coproduction with electricity was superior to electricity production alone. The VD/BIGCC combination had the highest process energy efficiency of 32.91% while the CHPSC-EE has the lowest energy efficiency of 15.44%. Regarding the economic comparison, it was seen that at the most conservative and optimistic pricing strategies, the ethanol production using VD/BIGCC had the highest internal rate of returns at 29.42 and 40.74% respectively.

Conclusions

It was shown that bioethanol coproduction from the hemicellulose fractions of sugarcane residues, with electricity cogeneration from cellulose and lignin, is more efficient and economically viable than the exclusive electricity generation technologies considered, under the constraints in a South African context.

Background

Sugarcane processing industries in Southern Africa generate bagasse at a yield of 0.30 tons per ton of cane processed[1]. In most sugar mills in Southern Africa, the generated bagasse is mostly burnt to provide heat and electricity for the sugar milling operations[1, 2]. South African sugar mills (from crushing to raw sugar production) typically have poor efficiency and the average steam demand is 0.58 tons per ton of sugarcane processed[3] (58% on cane). When such process designs are coupled with low efficiency biomass-to-energy conversion systems, then no surplus bagasse is generated by the sugar mill and therefore no export of electricity occurs[4, 5]. If efficient sugar mills that have steam demands below 40% [5, 6] are coupled with efficient systems that convert biomass to energy [6], then excess bagasse becomes available. This excess, if combined with other post-harvest residues like sugarcane trash, could provide the feedstock for the production of bio-energetic products in an integrated facility. The costs associated with the utilization of such residues would include the cost of collection and transport, and the investment costs required to upgrade the energy efficiency of existing sugar mills to enable the liberation of surplus bagasse. These costs are significantly lower than the purchasing costs of biomass[7] that hinders the economic viability of 'stand-alone' facilities for biomass conversion to energy[8].

The low efficiency biomass-to-energy systems in older cane milling operations utilized combustion systems that had raised steam to pressures of between 15 and 22 bar[5, 9]. Such systems also provided a low cost means of disposing of bagasse[1, 9] at a time

when exporting electricity was not economically interesting. For that means, combustion with high pressure steam cycles allowed for greater turbine efficiency in the conversion of steam to electricity and thus, pressures of 82 to 85 bar[1, 10] would have typically been preferred. At a pressure of 60 bar, it has been shown that a net electricity export of 72 kW/hr (per ton of cane processed) was possible for an efficient sugarcane mill, where a steam demand of 0.4 tons per ton of cane was required [5]. This amount of export electricity could have been increased substantially if the harvesting residues (trash) was also considered[5, 7, 11]. The electrical efficiencies resulting from biomass power plants utilizing combustion and high pressure steam cycles are reported to be between 23 and 26% on an HHV (Higher Heating Value) basis[12, 13], while efficiencies reported for Biomass Integrated Gasification and Combined Cycles system (BIGCC) were at 34 to 40%[14]. The implementation of BIGCC in industry has been limited due to the reportedly high capital investment that is required[12, 13, 15]. The capital estimates of BIGCC systems in previous techno-economic assessments[12, 13, 16] however, were based on the estimates in a period where BIGCC technology was still new (1990 to the early 2000s) [17], and thus, capital estimates based on the vendor quotes in this period would have reflected the pioneer plant costs. A capital estimate based on a matured estimate could be significantly lower than the pioneer estimate[18].

As an alternative to the conversion of all of the available lignocellulose residues to electricity, a fraction of the bagasse and post-harvest residues could be used to produce ethanol, with co-generation of electricity. The hemicellulose, which makes up about 20 to 35%[19] of the biomass matrix, can be solubilized by steam explosion or dilute acid hydrolysis and converted to ethanol, while the remaining cellulose-lignin fractions are

converted to heat and power[20, 21]. This scenario for the coproduction of ethanol and electricity from lignocellulose has been proposed for the South African industry[21], but a detailed process flow sheet and techno-economic investigation of such for existing sugar mills is not available. Of particular interest would be the techno-economic comparison of coproduction of ethanol and electricity against a scenario where the residues are used exclusively for electricity generation. Previous studies have compared electricity generation alone with the complete lignocellulose conversion to ethanol (hemicellulose and cellulose) as options for integration with sugar mills[22] and autonomous distilleries[7, 11]. The ethanol generation scheme in this study builds on the concept of 'value prior to combustion' that has previously been evaluated as a green-field (stand-alone) scenario[21].

There has been a considerable success in developing microbial strains that efficiently converts pentose-rich hydrolysates to ethanol[23], which is the key area of importance if the proposed technology is to be feasible. Using adapted strains of a the native pentose fermenting yeast *Pichia stipitis,* Kurian *et al*.[24] converted 82.5% of the hemicellulose sugars in a hydrolysate derived from sorghum bagasse that contained 92 g/l of dissolved sugars, while Nigam[25] converted 80.0% in an acid hydrolysate from wheat straw, containing 80 g/l sugars. The development of robust recombinant strains, such as the *Saccharomyces cerevisiae* TMB400, have resulted in pentose conversions in excess of 85% in toxic environments in simultaneous saccharification and fermentation experiments[26]. More recently, the National Renewable Energy Laboratory (NREL) achieved an ethanol yield of 92% on hemicellulose sugars in a toxic enzymatic hydrolysate that contained a total of about 150 g/l of sugars, using the *Zymomonas mobilis* strain that was genetically engineered

by Du Pont[27]. Thus, fermentation technology for converting pentose sugars in hydrolysates to ethanol has been successfully demonstrated on a laboratory scale.

The present study provides a detailed techno-economic comparison of scenarios that entail ethanol coproduction with export electricity, produced either by combustion or BIGCC systems, against those that produce only export electricity using the same systems. For either scenario, the upgrading costs of the existing sugar mill to achieve an energy efficiency of 0.40 ton of steam per ton of cane, is included in the capital investments considered in the economic analysis. The development of process models for the ethanol coproduction scenario will be based on established flow sheets and process performances for lignocellulosic ethanol[28, 29], and will also consider various processing options to ensure the most energy efficient and economical flow sheet. The projects are assumed to be in Kwa-Zulu Natal where the sugar cane crushing plants are concentrated. All South African legislations would apply. Energy efficiency for all of the scenarios will be maximized through pinch point analysis (PPA) for the heat integration of the processing streams[30–32]. This approach will ensure that the energy utilities for ethanol production are kept to a minimum[29, 30], consequently maximizing the export electricity while still providing the energy requirements of the (energy efficient) mill[33]. From the process simulations (mass- and energy-balances) for the various scenarios economic evaluations, incorporating capital and operational costs as well as sales prices, will be performed from an economic risk perspective[34–37]. These methods are based on Monte Carlo simulations that are super-imposed on standard methods for process economic methods, in order to account for the risks associated with the fluctuations in economic variables, thereby providing not only the estimates for investment returns, but also the probability of achieving economic success.

1 Methods

1.1 BASIS FOR SIMULATION AND ASSUMPTIONS

All of the scenarios analyzed in the present study assume that the steam demand of the sugar mill itself will be 0.4 tons per ton of cane processed The capital investments required to upgrade existing sugar mills in South Africa to achieve this level of energy efficiency has been estimated at US$ 17.32 million[3, 38] [3, 47] (in 2012) for a 300 ton per hour crushing rate. The technical measures include**d** the optimisation of imbibitions rate to reduce the amount of evaporation needed[38]; the conversion from the batch pans to continuous pans and reduce the pan movement water[3, 9, 38]; using a five-effect evaporator where vapour is bled to the vacuum pans at a lower effect[9]; optimisation of the flashing of condensates for steam recovery[38] and finally; electrifying the turbine drivers[3, 4].

The cane crushing capacities of mills in South Africa range from 190 to 600 tons per hour [39, 40], and thus the representative average of 300 tons per hour was assumed for the present study. Based on a fibre content of 0.14 kg/kg of cane[5], 42 tons per hour of bagasse would be generated from the cane crushing activities for energy generation. Of the total harvesting residues, amounting to 1.167 kg per kg of bagasse[41], 50% of this amount would be collected and co-fed with all the bagasse into an ‘energy island’ in the mill to generate the energy requirements of the mill (40% steam on cane[42] and 41.64 kWe[4] per ton of cane) and the export energy products. The composition of the residues is shown in Table 2.

Table 2: Chemical composition of sugarcane residues

Component (%)	Bagasse[1]	Trash[2]
Cellulose	41.1	39.8
Hemicelluloses	26.4	28.6
Lignin	21.7	22.5
Ash	4.0	2.4
Extractives	6.8	6.7

1. Average of measurements for South African bagasse[43, 44]
2. Composition taken Oliveira *et al*.[45]

1.2 PROCESS TECHNOLOGY CONSIDERATIONS

1.2.1 Exclusive electricity generation from lignocellulosic biomass

Nsaful *et al.*[42] developed a flow sheet for the conversion of bagasse from a sugarcane milling operation to steam and electricity with a high pressure steam system using combustion (Figure 6). They found that the optimum boiler pressure for efficient electricity generation was 82 bar. Based on the net amount of export electricity, the electrical generation efficiency was 21.5% for 82 bar and 20% for 63 bar. Conversations with experts in the South African sugar industry indicate that the design pressure for boilers which will be used to retrofit the sugar mills is 86 bar. Consequently, a boiler pressure of 86 bar is assumed in this study. Conventionally, biomass would enter the combustor at about 45% moisture, though it could also be dried with flue gas to improve the boiler efficiency, with additional capital charges. The minimum acceptable moisture content for bagasse is 30%, so as to avoid self-ignition and/or a dust explosion[46]. Excess air is provided to the boiler, which has been preheated to 250°C [42] by the stack gas, to improve the overall efficiency. The amount of air in excess is determined to ensure a minimum oxygen content of 6% in the flue gas, as per environmental regulations[47].

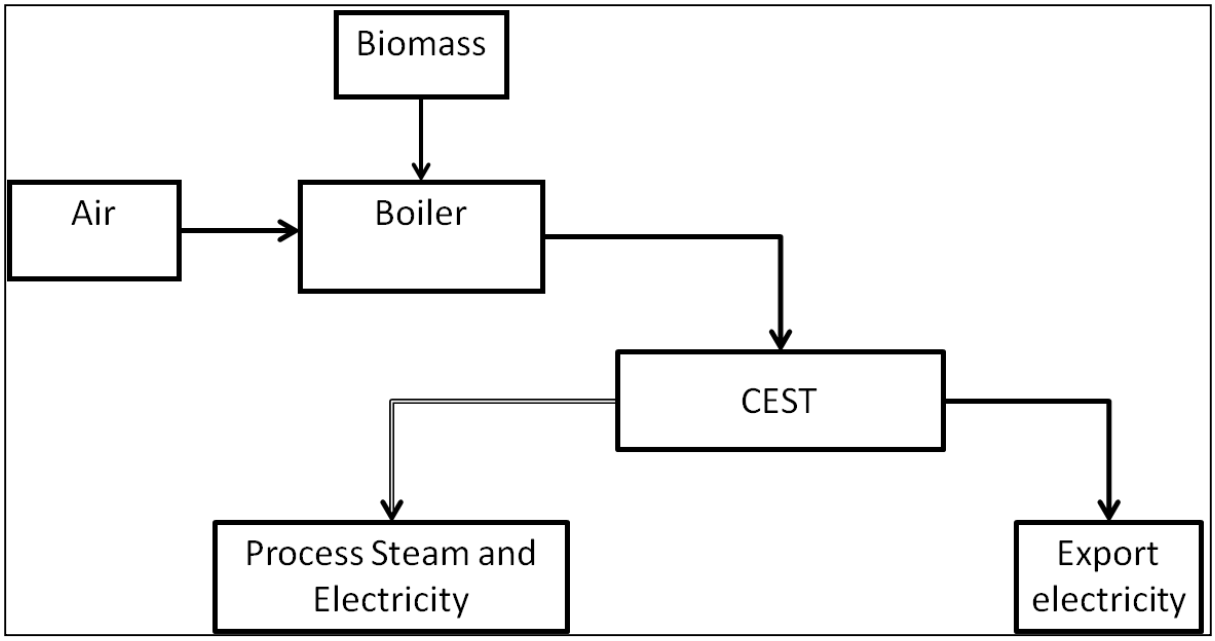


Figure 6: Combustion with High Pressure Steam cycles (CHPSC) flow sheet. (CEST – Condensing Extraction Steam Turbine)

The boiler would generate superheated steam at about 515°C [10] and 86 bar that would be expanded in a CEST to generate electricity. The intermediate pressures in the CEST are 13 and 4 bar, and the final vacuum pressure is 0.2 bar[48]. The vacuum steam would then be condensed and returned to the steam cycle. Steam for the mill would be extracted from the CEST at 4 bar. Regarding the performance of the turbines, the isentropic efficiency was 85% while the combined mechanical and electrical efficiencies were set at 96.06% (i.e. 98% for electrical and 98% for mechanical)[49].

The general flow sheet of the BIGCC system (Figure 7) for biomass conversion to electricity was adapted from models developed by the NREL[50, 51] and previous reports[52–54]. The combined bagasse and trash would be initially dried to a moisture content of 10 to 15% with exhaust flue gasses[52, 53]. The moisture content within the biomass would serve as the gasification control agent[52] since steam injection is generally not considered for gasifier applications in the BIGCC systems. The amount of air added to

the circulating fluidized bed (CFB) gasifier in the BIGCC system is to ensure the highest possible calorific value of the syngas without an excess of tars. To initiate tar cracking, the gasifier is required to be operated at 800°C. This is achievable when the ratio of the air supplied to the stoichiometric amount for complete combustion (equivalence ratio) is 0.25 to 0.3 [52]. The syngas would then enter a cyclone to remove particulate matter before entering the CFB tar cracker, where additional air is added to increase the temperature to 920°C for cracking to occur with a dolomite catalyst[51].

After tar cracking, the temperature of the syngas would be reduced to 288°C in order to condense the alkali species for removal with any other particulate matter in a filter bag [46]. The syngas is further cooled to 97°C before it is scrubbed with water to remove the nitrogenous and sulfurous compounds for the protection of downstream equipment, and to prevent nitrous and sulfurous oxide emissions[51, 53]. The scrubbing also humidifies the syngas, which assists in the control of the temperature in the gas turbine[55].

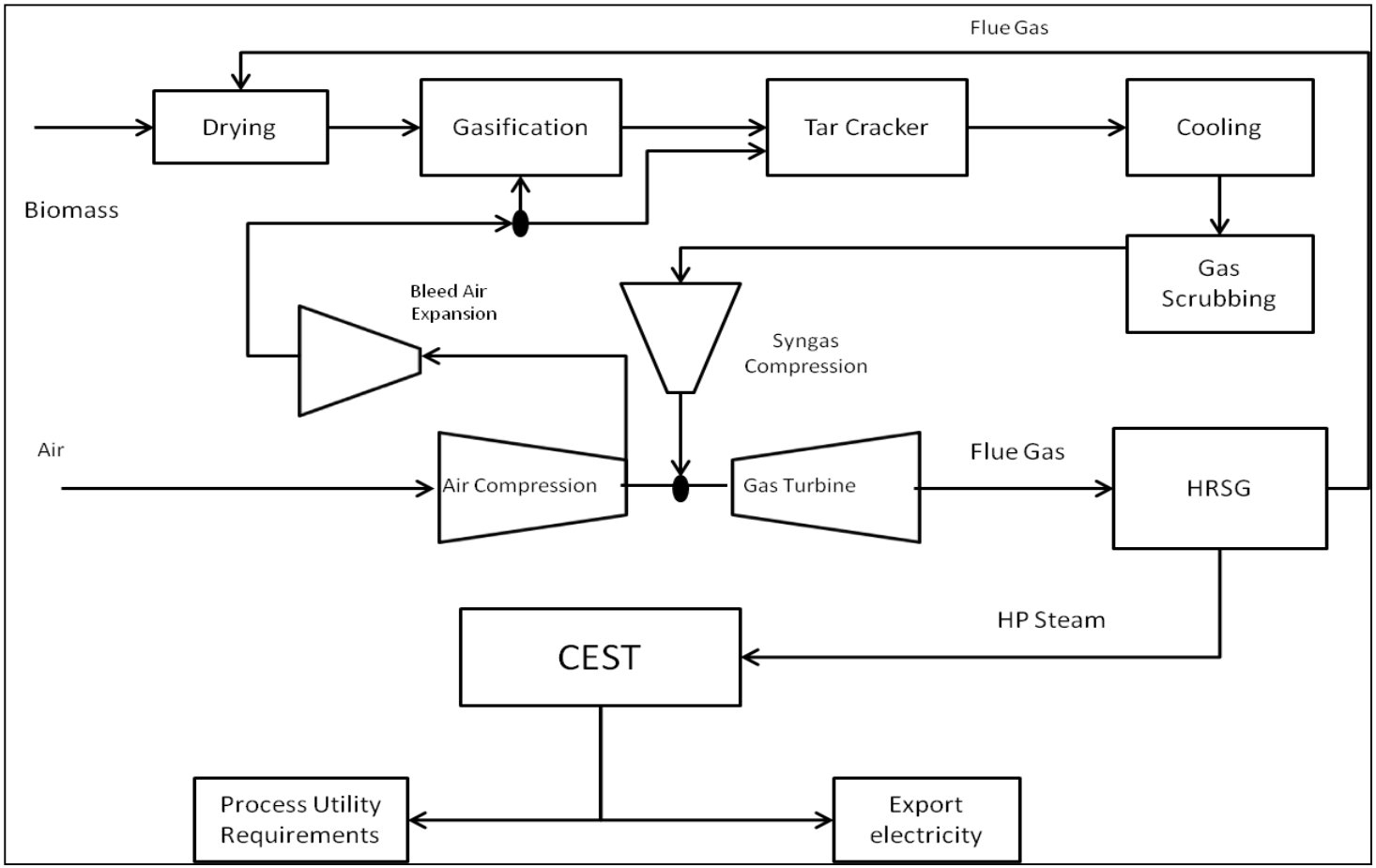


Figure 7: Biomass Integrated Gasification and Combined Cycle flow sheet. (CEST – Condensing Extraction Steam Turbine; HRSG – Heat Recovery Steam Generator; HP Steam – High Pressure Steam)

The syngas is compressed in a multi-stage compressor (two compressors with an inter-stage cooler in-between) to 20 bar, which is 4 bar above the combustion pressure of the gas turbine[56], in order to allow for the pressure drop across the feed nozzle[50]. At the inter-stage cooler, the syngas was cooled to 97°C at an intermediate pressure of 6 bar, which was determined by the optimization procedure of Polyzakis *et al.* [56]. The air required for the gas turbine would be compressed in the compressor chamber of the gas turbine, and is fed at a mass ratio of 1:5.14 to the syngas[57]. In order to compensate for the extra volumes of dilution gasses in the syngas that is not found in natural gas, such as CO_2 and nitrogen, air would be bled from the compressor chamber before the air enters the combustion chamber[51, 53, 57] since the gas turbines are designed for natural gas which does not contain inert gasses. The rate at which air is bled amounts to 13.3% of the air fed to the compression chamber, which is in excess of the air demands of the gasifier and cracker. The bleed air would be expanded through a turbine to atmospheric pressure to improve the net electricity output[53]. Once expanded, the air would be preheated to the gasifier temperature to be used to feed the gasifier and tar cracker. Regarding the efficiency of the gas turbine, the compressor section has a polytrophic efficiency of 87% and the gas turbine has an isentropic efficiency of 89.77%[49]. The mechanical and electrical efficiencies are both set at 98% [49].

The combustion exhaust gas leaves the combustion chamber at about 1100°C and is expanded to 1 bar in the turbine section to generate the bulk of the electrical output by driving the generator. The heat of exhaust gasses of the turbine is captured in a HRSG to generate steam at 60 bar for the 'combined' steam cycle[50, 53, 54]. The superheated

steam is generated with water that had been preheated with waste heats from the BIGCC system, as determined by PPA. The superheated steam is then expanded in a CEST to provide the steam demands and additional electricity. The exhaust gas of the HRSG has a temperature of 200°C and is used to dry the biomass that entered the BIGCC system[53].

1.2.2 Ethanol coproduction from hemicellulose

A general overview of the process flow sheet for the coproduction of ethanol and electricity is presented in Figure 8. Regarding the process step for pre-treating the biomass for hemicellulose solubilisation, the two methods that have been established for this purpose are dilute acid hydrolysis (DAH) and steam explosion (STEX). As shown in Table 3, the DAH process typically provided a lower yield of hemicellulose sugars than the STEX and only operated effectively at solid contents of 20% and below. STEX had been shown to operate effectively at 50% (Table 3), which implies that the energy requirements for DAH were much higher due to the large volumes of water to be evaporated to concentrate the hydrolysate for efficient downstream processing[43, 58]. Thus, STEX was selected as the technology for hemicellulose solubilization. After pretreatment, the pretreated slurry is washed and filtered to recover the solubilized sugars as a filtrate from the solid residue (containing the cellulose and lignin fractions) that is converted to heat and power (via CHPSC or BIGCC). The sugar recovery to the filtrate was conservatively estimated at 80%, even though recoveries as high as 91% have been reported in the literature[21]. Regarding the gasification of residue from steam explosion, it produces a syngas with a higher calorific value than that produced from raw biomass, but the gasifier must be slightly bigger, to accommodate the lower reactivity of the pretreated biomass[59].

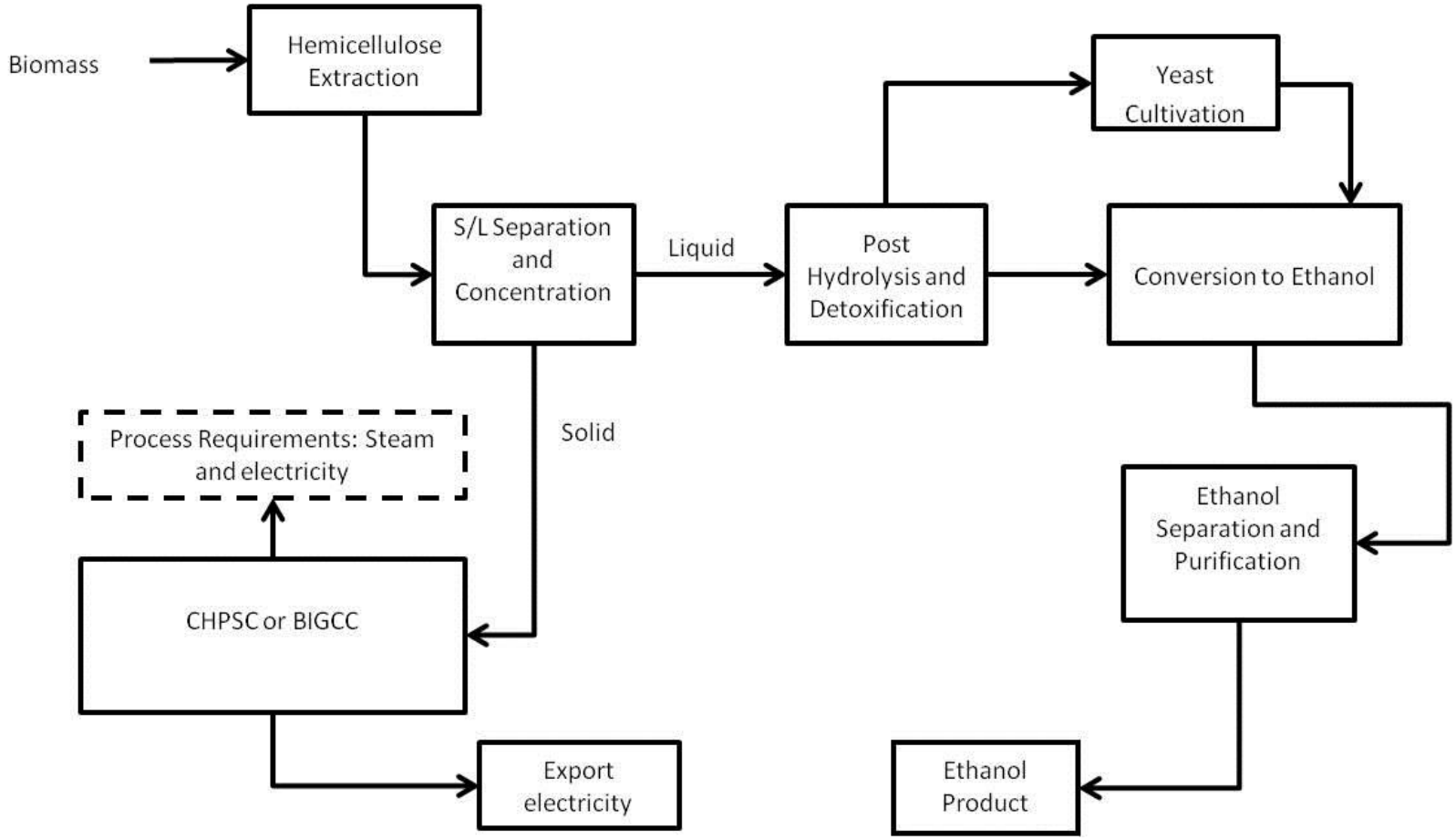


Figure 8: Ethanol coproduction flow sheet. (BIGCC - Biomass Integrated Gasification and Combined Cycles system; CHPSC – Combustion with High Pressure Steam Cycle; S/L Separation – Solid Liquid Separation

Table 3: Comparison of hemicellulose solubilization techniques (WIS – Water insoluble solids)

Dilute Acid Hydrolysis				
	Hemicellulose	**WIS**	**Solubilisation**	**Yield**
	%	**%**	**%**	**g/100 g**
Aguilar et al.[60]	21	10	92	19.0
Canilha et al. [19]	26	-	62	15.9
Tricket [61]	30	19	71	21.3
Diedericks et al. [44]	24	30	75	18
Lavarack et al. [62]	28	20	72	20.0
Steam Explosion				
Rudolf et al. [26] (SO_2 catalysed)	26	50	87	23
Carrasco et al. [63](SO_2 catalysed)	24	50	57	16
Ferreira-Leitao et al. [64](CO_2 catalysed)	23	50	63	14
Laser et al. [65](uncatalysed)	26	50	91	24
Rocha et al. [66] (uncatalysed)	25	50	82	21
Oliveira et al. [45] (uncatalysed) (trash)	29	85	93	27

Table 4: Fermentation parameters

Parameter	**Value and Description**
Hydrolysate	Alkaline detoxification [24, 25]
Total dissolved sugars in raw hydrolysate	200 g/l primarily consisting of pentose, originating as 88% of the hemicellulose converted. Glucose originating from 30% solubilisation of the cellulose in the trash [45]
Fermentation Mode	Fed-batch, initially with 60% of the reactor loaded with diluted hydrolysate
Fed-Batch Initial Sugars	92 g/l, as per the hydrolysate in Kurian et al.[24]
Yeast loading	1.5-2 g/l dry weight [25, 27]
Conversion to Ethanol	82.5% of pentose, 90% of hexose
Fermentation Time	140 hours [67]
Temperature	30^{o}C, temperature maintained with a chiller.

STEX without catalysis requires a secondary hydrolysis of the hydrolysate to convert the oligomers to fermentable monomeric sugars[68] by treatment with sulfuric acid at a level of 0.5% (wt) in solution at 120°C for 20 minutes [68]. This two-step process is advantageous over the catalyzed STEX (and DAH) because catalysis is intended for improving enzymatic digestibility (which is of no significance in this study) rather than the solubilisation of hemicellulose [69]. Furthermore, the yield of solubilisation with no catalysis is less variable, as shown in Table 3 and lastly, the costs of purchasing or producing SO_2 and effective impregnation equipment are avoided.

The theoretical conversion of hemicellulose of the mixed biomass is assumed as 88% (wt.), which is the weighted average obtained with bagasse[65, 66] and trash [45] (at a feed ratio of 1:0.583) at temperatures ranging from 200 to 210°C with a STEX time of 10 minutes. At such conditions the formation of degradation compounds is significant enough to inhibit the fermentation organisms[65], and thus the neutralization of these compounds by detoxification is necessary. The mode of detoxification would be alkaline treatment[24, 25, 28] at temperatures below 30°C so that no sugar loss occurs[70]. While detoxification has been criticized as an unnecessary economic hurdle in previous process evaluations, it has been shown experimentally that detoxification improves the yield of fermentation by 20 to 25%, even if inhibitor resistant strains are used[25, 71]. In this study, ammonium hydroxide will be used to carry out detoxification[72] in order to avoid the environmental and operational issues associated with over-liming. The yield of ethanol on sugar and other fermentation parameters for the present study are presented in Table 4, which are conservatively assumed based on previous performances in literature[26, 73]. To ensure this yield, fed-batch fermentation is adopted, since this mode of fermentation can be 1.5 times

more efficient than batch fermentation[74]. With regards to the hexose sugars, which resulted primarily from the cellulose content of the sugarcane trash, the conversion will be assumed as 90% since the yeasts consume these sugars at a much faster rate than the pentose sugars[25].

After fermentation, the beer product is purified in the refining section to produce anhydrous ethanol. The beer is initially flashed at 86°C and 0.83 bar to remove the carbon dioxide (CO_2), and the flash gas enters a knockout drum at 1.1 bar to condense ethanol that has evaporated[43, 58, 75]. The gas from the knockout drum is then combined with the fermentation vent stream and enters a scrubber to ensure the maximum recovery of ethanol[43, 58, 75]. The effluents from the scrubber and knockout drum are combined with the beer stream from the initial flash and fed to the beer column, which produces a vapor phlegm [29] that contains ethanol at 40 to 50%. The phlegm is then fed to a rectifier column that produces hydrous ethanol phlegm of 91%[75]. The hydrous ethanol phlegm is dehydrated by molecular sieves to produce ultra-pure ethanol product of 99.7%[43, 58, 75].

In a variation of the configuration described, the beer column can operate at a vacuum pressure of 0.2 bar, which allows for the heat required by the reboiler of beer column to be supplied by the condenser of the rectifier. Dias *et al.* [29] had shown through pinch-point heat integration that the steam demand of the refining section of an ethanol distillery can be significantly reduced if such a strategy is employed. This variant would, however, require a vacuum pump to actuate, which implies that the economic impacts of the lower steam demand would need weighing-up with the higher electricity and capital requirement.

1.3 SCENARIO DEVELOPMENT AND SIMULATION

1.3.1 Development of scenarios

For electricity and steam generation, technological variants included biomass integrated gasification with combined cycles (BIGCC) and combustion with high pressure steam cycles (CHPSC). Regarding ethanol purification, the technological variants included conventional distillation (CD) and vacuum distillation (VD). Therefore, from these process technologies, the alternative process scenarios that were modelled as all possible combinations of the process options included BIGCC exclusive electricity generation (BIGCC-EE); CHPSC exclusive electricity generation (CHPSC-EE); CD/BIGCC for coproduction of ethanol and electricity; CD/CHPSC for coproduction of ethanol and electricity; VD/BIGCC for coproduction of ethanol and electricity and VD/CHPSC for coproduction of ethanol and electricity.

1.4 TECHNICAL SIMULATION

The simulation of all scenarios were completed in Aspen Plus® (Aspen Technology, Inc., Massachusetts, USA) [76] by modelling the flow sheets with the relevant design parameters discussed in the section dealing with process technology considerations. Reactors were simulated as the stoichiometric reactor 'RSTOIC' using conversions evaluated from available experimental data[28, 37, 43, 58]. The gasifier in the BIGCC scenarios was modelled as a combination of an adiabatic combustor and equilibrium reactor that determines that determines the gas composition by minimizing the Gibbs Free Energy 'RGIBBS', since the composition of the syngas is close to the equilibrium values[51, 52, 77, 78]. Regarding thermodynamic properties, the Non-Random Two-Liquid model (NRTL) for electrolyte systems (ELECNRTL) was used whenever there were electrolytes to consider, and the NRLT was used to model the separation systems[29, 43].

The utility requirements were determined with PPA, by importing heat duties of streams and flash drums determined by the Aspen Plus® simulations into the IChemE pinch analysis spreadsheet[79] which were used to calculate the hot and cold utilities according to the methods of Kemp[31] and March[32]. The hot utility would also be supplied using the low pressure steam from the CEST at 4 bar, while the cooling utilities are achieved through cooling towers. After the utility requirements were taken into account, the net export efficiency (η) was calculated as the combination of the net export of electricity (E_{net}) and calorific value of the ethanol fuel (F) relative to the calorific input of the biomass ($m*HHV_{biomass}$), as shown in Equation 1 (the standard unit used for these energy quantities was MJ/hr).

$$\eta = \frac{E_{net} + F}{m \times HHV_{biomass}} \quad \text{(Equation 1)}$$

1.5 FINANCIAL RISK ASSESSMENT

1.5.1 Method and assumptions

Results from the process models were used in the economic evaluation models for each of the scenarios considered, in accordance with established process evaluation techniques[80]. The information emanating from these models were used to calculate the key economic variable (KEI), namely, IRR[80]. A Monte Carlo simulation was super-imposed on the financial evaluation models in order to create a financial risk assessment whereby the input of certain economic variables into the financial statements would be based on probabilistic distributions that are determined by historical data. This process is then repeated for a large number of iterations and the KEIs generated from the iterations are stored for aggregation in a statistical assessment. The methods followed for these

simulations have been described in detail by Richardson et al.[34, 35, 81] and by the authors of the current study[36, 37]. The software used for carrying out the simulation was the Simetar Risk Analysis Software (Simetar, Inc., Texas, USA) [82]. The economic parameters that define a South African context under which the financial risk of all processing scenarios were evaluated are given in Table 5.

Table 5: Boundary Parameters for Economic Evaluation

Parameter	Description
Plant Life[43]	25 years, with 9 operational months per year. The salvaging value is 20%.
Period of Economic Analysis[37]	20 years
Depreciation[37, 43]	Straight line to salvaging value.
Tax [35]	South African company tax of 28%
Working Capital[43]	5%
Other	To simplify the analysis, an equity of 100% was assumed[28, 43]. It was further assumed that capital will be fully paid after construction.

1.5.2 Capital cost estimates

The capital costs of generic equipment such as pumps, process drums and turbines were predicted with the Aspen Icarus® (Aspen Technology, Inc., Massachusetts, USA) estimator. For all the major or specialized equipment in the ethanol process model, the costs were based on vendor and literature based quotes, such as those in Humbird *et al.*[27] for steam explosion, hydrolysis equipment and filter presses; Aden *et al.*[28] for detoxification equipment, cooling water mains pump and cooling tower system; Bailey[83] for surface condensers; Ridgway[84] for vacuum pump; Al-Riyami *et al.*[85] for heat exchanger costs and finally, Craig and Mann[51] for flue gas biomass dryer.

The cost of the high pressure boiler systems was provided by experts in the South African sugar industry. However, for the BIGCC it was seen that capital estimates tended to be based on whole plant costs in the literature[16, 86]. Many of these estimates could be traced to vendor quotes from the period when the costs of BIGCC systems were still pioneer costs[13, 16, 86]. Therefore, the most relevant estimate was found in the representative costs in the Report on Combined Heat and Power, of the Environmental Protection Agency of the USA (EPA CHP)[87], which was based on vendor quotes of modern equipment costs.

1.5.3 Nominal economic variables

In this study, nominal economic variables' refers to specific prices and indices that form the basis of operating costs, incomes and interest-based transactions. These specific values were either determined from the literature or from published databases and are listed in Tables 7 and 8. The variables are treated as 'static' variables (Table 6), which means that the basic prices in year one of the assessment was taken as an average value estimates and inflated with the projected Producers Purchases Index (PPI) to predict the future value. The 'stochastic' variables (Table 7) were used to generate a multivariate empirical function, from which the future values were iteratively projected for each year in the evaluation in the Monte Carlo simulation.

Table 6: Static nominal economic expenses

Item	Cost Basis**	Value
Maintenance and Repair[35]	US$/litre	0.004
Labour Ethanol plant [35]	US$/litre	0.016
Management and Quality Control[35]	US$/litre	0.005
Real Estate Taxes[35]	US$/litre	0.001
Licenses, Fees and Insurance [35]	US$/litre	0.001
Miscellaneous Expenses[35]	US$/litre	0.005
Total Chemical Cost (per annum)	US$	2, 850, 292
CHPSC Operating Costs[87]	US$/kWhr	0.007
BIGCC Operating Costs [87]	US$/kWhr	0.013
Trash Price[7]	US$/dry ton	20.44

Bagasse Price [1]	US$/dry ton	6.3

**All prices are given for the year 2012 in the South African Market

[1] Amortized cost for upgrading a South African mill to 40% steam on cane for liberating bagasse.

Table 7: Database for stochastic variables

	Electricity [88]	**Brazilian Ethanol** [89]	**USA Ethanol** [90, 91]	**PPI** [92]	**Interest Rate** [93]
Unit	US$ per kWhr	US$/litre	US$/litre		%
2003	0.032	0.252	0.337	124.80	15.16
2004	0.039	0.254	0.422	127.70	11.31
2005	0.044	0.375	0.463	132.40	10.64
2006	0.048	0.508	0.674	142.60	11.14
2007	0.040	0.467	0.524	158.20	13.08
2008	0.040	0.520	0.587	180.80	15.12
2009	0.045	0.450	0.449	180.70	11.80
2010	0.054	0.612	0.483	191.60	9.91
2011	0.087	0.867	0.683	207.60	9.00
2012	0.106	0.666	0.611	220.50	8.78

Regarding the price of second generation ethanol, uncertainty exists because the current pricing of the South African biofuel strategy does not explicitly include second generation fuels[94]. Thus, the price of ethanol was either based on data given for ethanol prices in the USA, or based on data describing Brazilian (BRZ) ethanol prices. Given the uncertainty in the selling price of the export electricity, an upper and lower premium was calculated and applied on the base electricity prices projected from the probability distribution. These premiums were calculated on the minimum and maximum prices for renewable electricity of the South African Renewable Energy bids, which had 2012 based prices of 0.113 and 0.175 US$ per kW/hr respectively[95]. Since biomass based energy is

continuous and supplies energy for peak hours, a bonus price of two times the renewable energy price is allowed for four hours per day[95], which thus raises the average renewable prices to 0.139 and 0.216 US$ per kW/hr. Relative to the base electricity price (2012 price) in Table 8, the upper and lower premiums amount to 31% and 103% respectively.

With the two possible renewable electricity premiums and two sets of ethanol price data, there would be four possible pricing strategies. Each strategy is considered as a set of parameters under which separate sets of stochastic evaluations of the process scenarios will be conducted. These four pricing strategies are: 1) minimum electricity premium and ethanol prices based on Brazilian data, 2) minimum electricity premium and ethanol prices based on USA data, 3) maximum electricity premium and ethanol prices based on Brazilian data, and 4) maximum electricity premium and ethanol prices based on USA data.

1.6 SENSITIVITY ANALYSIS

The modern capital estimates of BIGCC carry some uncertainty, in that they might be too optimistic. Thus, in order to account for the possibility of a more pessimistic capital estimate, the capital estimate of the BIGCC power plant equipment was increased by 10%, prior to factoring in balance of plant costs (BOP) and project contingencies. Accordingly, a separate stochastic simulation of the BIGCC-EE, CD/BIGCC and VD/BIGCC scenarios was carried out to evaluate the impact of the pessimistic capital estimate.

There is also uncertainty in the yield of ethanol from the hydrolysate, as a very sophisticated organism could yield more ethanol without the need for detoxification, hence negating the associated costs. Furthermore, it is also possible that suboptimal hemicellulose extraction could result in a loss of ethanol. Thus, two sensitivity scenarios of the most

profitable coproduction scenarios were simulated. They include: (1) where the overall ethanol yield is decreased by 10% to account for the suboptimal hemicellulose extraction, and (2) where the overall ethanol yield is increased by 10% to account for a possibility of a sophisticated fermenting organism which will further discard the costs associated with detoxification. Accordingly, the economic sensitivity to these variations in process parameters was determined using separate stochastic evaluations.

2 Results and Discussion

2.1 TECHNICAL EVALUATION

Six scenarios for the production of electricity from sugarcane residues, either as the only energy product or with coproduction of ethanol from hemicellulose, were evaluated through process modelling to estimate process energy efficiency and economics. The results of the energy characteristics for the various process alternatives that have been optimized by pinch point analysis are presented in Table 8. Furthermore, the amount of steam generated by the heat and power facility in each scenario, whether this facility forms an exclusive electricity scenario or an energy generation section of an ethanol coproduction scenario, is presented. If the facility utilizes the Combustion with High Pressure Steam Cycles (CHPSC) technology, then the gross steam generation refers to gross amount of steam generated by the biomass-fired boiler. If the heat and power plant utilizes the BIGCC technology then the gross steam generation refers to the steam generated by the heat recovery steam generator (HRSG) that recovers heat from the gas turbine's exhaust. The steam contingency refers to the amount of steam that is reserved once all the demands of the sugar mill and ethanol plants (in the case of ethanol coproduction scenarios) are met, and is essentially an indication of the operating leeway the scenario offers in terms of

meeting steam when fluctuations in the plant occur. According to Pellegrini *et al*.[96], the maximum fluctuation of the steam demand in a sugar mill was measured at 2%.

The ethanol production rate of all the coproduction scenarios averages 9591 l/hr, which would equate to 62 million liters per annum. Given that the total consumption of road transport fuel in South Africa is about 23 billion liters per annum[97], this production rate would represent 0.27% of road transport fuels. This production rate equates to an ethanol yield of 35 liters per ton of cane crushed, where the hemicellulose fraction of the bagasse and 50% of the trash generated is converted to ethanol. With regards to the exclusive electricity generation, the BIGCC-EE and CHPSC-EE (EE - exclusive electricity production using BIGCC and CHPSC respectively) scenarios generated 88.63 MW and 53.43 ±2.43 MW of electricity (MWe) respectively. Given that the total output of electricity supplied to the national grid is 34 GW[98], then the contribution to the grid would be 0.26% and 0.13% for the BIGCC-EE and CHPSC-EE respectively. The coproduction of ethanol with electricity from sugarcane residues available at sugar mills would reduce the potential electrical export by approximately 54% on average.

With regards to the steam generation and demand, it is seen that the gross generation of steam in the BIGCC-EE process is 32.86% less than the amount of the CHPSC-EE process, primarily because BIGCC technology is meant to maximize electricity generation, rather than steam generation. The steam generated by the heat and power generation facilities of the ethanol coproduction scenarios are 28.4% lower when compared to their exclusive electricity counterparts. The major implication of this reduction for steam generation was that when BIGCC technology was coupled with ethanol coproduction, the combined steam demand of the sugar mill and the ethanol generation process exceeded the

steam generated. This penalized the electricity generated by the ethanol-BIGCC scenarios, as electricity was needed internally for heating purposes, at a rate of 2.43 MW and 15.63 MW for the VD/BIGCC and CD/BIGCC respectively. Thus, the vacuum distillation scenarios offered a more feasible operating scenario when BIGCC technology was considered, as the lower steam consumption minimized the electricity consumed for heating purposes.

Table 8: Bio-energetic product yields, utility demands and energy efficiencies (optimized by pinch point analysis)

	Ethanol Cogeneration				Exclusive electricity		
Scenarios	**CD/CHPSC**	**CD/BIGCC**	**VD/CHPSC**	**VD/BIGCC**	**CHPSC-EE**	**CHPSC –EE (Dryer)**	**BIGCC-EE**
Net Outputs							
Bioethanol Production (l/hr)	9601	9577	9599	9575			
Electricity Production (MW)	22.06	33.94	23.42	46.47	51.00	55.85	88.63
Steam Generation and Requirements							
Gross Steam Generation (tons/hr)	204.58	146.43	204.58	146.42	277.22	294.71	191.98
Mill Steam Demand (tons/hr)	120.00	120.00	120.00	120.00	120.00	120.00	120.00
Ethanol Generation Steam Demand (tons/hr)	51.06	51.06	30.25	30.25			
Steam Contingency (tons/hr)	33.53	−24.63	54.34	−3.83	157.22	174.71	71.98
As percentage of Total Steam Demand	19.60	−14.40	36.17	−2.55	131.02	145.59	59.99
Electricity Generation and Requirements							
Gross Electricity Generation (MW)	38.52	187.50	40.76	187.51	65.49	70.50	263.36
Power Utilities (MW)	1.17	122.63	1.36	122.63	2.00	2.15	162.24
Ethanol Utilities (MW)	2.81	18.44	3.49	5.91			
Mill Electricity Demand (MW)	12.49	12.49	12.49	12.49	12.49	12.49	12.49

Net Energy Efficiency	**25.57%**	**29.17%**	**25.98%**	**32.91%**	**15.44%**	**16.86%**	**26.83%**

A further comparison of vacuum and conventional distillation shows that the application of vacuum distillation allowed for an extra 1.36 MW of electricity to be available for export (comparing CD/CHPSC and VD/CHPSC). This was because the lower steam demand of the vacuum distillation system on the steam utilities allowed for more steam to expand through the exhaust steam turbine of the condensing extraction steam turbine (CEST). Furthermore, the multi-effect system also relieved the cooling duty of the condenser of the rectifier column, and thus, no further electricity was needed to deliver this cooling duty. So even though there was an additional process electricity requirement for the vacuum pump that actuated the multi-effect distillation, the reduction in utility requirements exceeded the requirement, which then resulted in a net positive electricity export.

The energy efficiencies reported in Table 8 were based on the net export of the bio-energetic products, which is the ethanol sold and the electricity exported to the grid after the mill requirements were accounted for. Generally, ethanol scenarios with BIGCC technology had the greatest net export efficiency, followed by that of the BIGCC-EE, which was comparable to the ethanol-CHPSC scenarios, and the lowest being the CHPSC-EE scenario. The reduction in steam consumption in vacuum distillation when CHPSC and BIGCC technology are used for energy generation is shown to improve the export electricity efficiency by 0.41% and 3.74% respectively. The improvement when BIGCC technology was integrated with vacuum distillation is explained by the lower amount of electricity consumed internally for heating purposes. The lowest export energy efficiency was attained by the CHPSC-EE scenario, due to the large amount of exhaust steam still present after the steam demand of the sugar mill was accounted for. The energy contained in this steam is

mostly spent to the environment by the surface condenser. If a biomass dryer was used to de-moisture the biomass prior to combustion, as in the case of the CHPSC-EE, then the export efficiency improved by 1.42% because the steam and electricity generation had improved by 6.14% and 7.65% respectively.

In order to assess the benefits of pinch point analysis (PPA), values are compared with the corresponding values in Table 9. Table 9 does not report values for the exclusive electricity scenarios because effective heat integration is implicit in the overall design of these processes. Regarding the CHPSC-EE, the design of Nsaful *et al.*[42], which is the source model for the CHPSC technology, was already optimized with PPA. As for the BIGCC-EE, PPA confirmed the heat integration strategies that have previously been implemented, such as the cooling of the syngas to heat up air for the gasifier, improving steam generation, and also using the inter-cooler duty of the multistage compressor to improve steam generation[37].

Table 9: Yields, utility demands and energy efficiencies without pinch point analysis

Scenarios	CD/CHPSC	CD/BIGCC	VD/CHPSC	VD/BIGCC
Net Outputs				
Bioethanol Production (l/hr)	9601	9577	9600	9575
Electricity Production (MW)	18.63	21.09	20.37	32.78
Steam Generation and Requirements				
Gross Steam Generation (tons/hr)	204.58	146.43	204.58	146.42
Mill Steam Demand (tons/hr)	120.00	120.00	120.00	120.00
Ethanol Generation Steam Demand (tons/hr)	68.62	68.62	49.56	49.56
Steam Contingency (tons/hr)	15.97	−42.19	35.02	−23.14
As percentage of Total Steam Demand	8.47	−22.37	20.66	−13.65
Electricity Generation and Requirements				
Gross Electricity Generation (MW)	36.63	187.50	38.99	187.51
Power (MW)	1.01	122.63	1.21	122.63

Ethanol Utilities (MW)	4.50	31.29	4.92	19.61
Mill Electricity Demand (MW)	12.49	12.49	12.49	12.49
Net Energy Efficiency	24.53%	25.23%	25.05%	28.76%

The comparison between Table 8 and Table 9 shows that the potential for exporting electricity from the ethanol-BIGCC scenarios are reduced by a margin of 30 to 38% if PPA is not applied, mainly because the increase in steam demand resulted in more electricity consumed for heating purposes. Thus, the primary advantage of PPA is the reduction of steam and electrical utilities, which then resulted in the net export of more electricity, and the general increase in the export energy efficiencies by 0.98 and 4.04 percentage points for ethanol-CHPSC and ethanol-BIGCC scenarios respectively. The effect of PPA on the scenario employing conventional distillation seems more apparent because the vacuum distillation already affected a substantial reduction in utilities by inducing multi-effect distillation.

2.2 ECONOMIC RESULTS

The six scenarios for the production of electricity from sugarcane residues, either as the only energy product or with coproduction of ethanol from hemicellulose, were compared in terms of the total capital investments (TCI) required (Figure 9), the economic viabilities in terms of internal rates of return (IRR) on the investments (Figure 10), and the financial risk of each investment, based on the Monte Carlo simulation, quantified as the probability of an acceptable return on investment (Figure 11). Figure 9 shows that the highest capital investment was 324.57million US$ for the VD/BIGCC cogeneration scenario, which was also the scenario with the highest energy efficiency. The primary reason for the high capital investment is the costs associated with the integrated BIGCC, as shown by the difference in capital costs between the ethanol scenarios with vacuum distillation that have

either the CHPSC or BIGCC technologies integrated as energy islands. The application of the vacuum distillation also demanded higher capital costs, as is shown by the general comparison of the vacuum and conventional distillation scenarios. With VD, additional capital charges were also incurred by the larger capacity of the surface condenser and circulation pumps. This was because of the lower steam demand, which resulted in a greater throughput of steam in the equipment mentioned. Thus, the use of VD is shown to increase the capital expenditure by 9.33% when CHPSC technology is used, and 4.33% when the BIGCC technology is used as energy schemes, respectively.

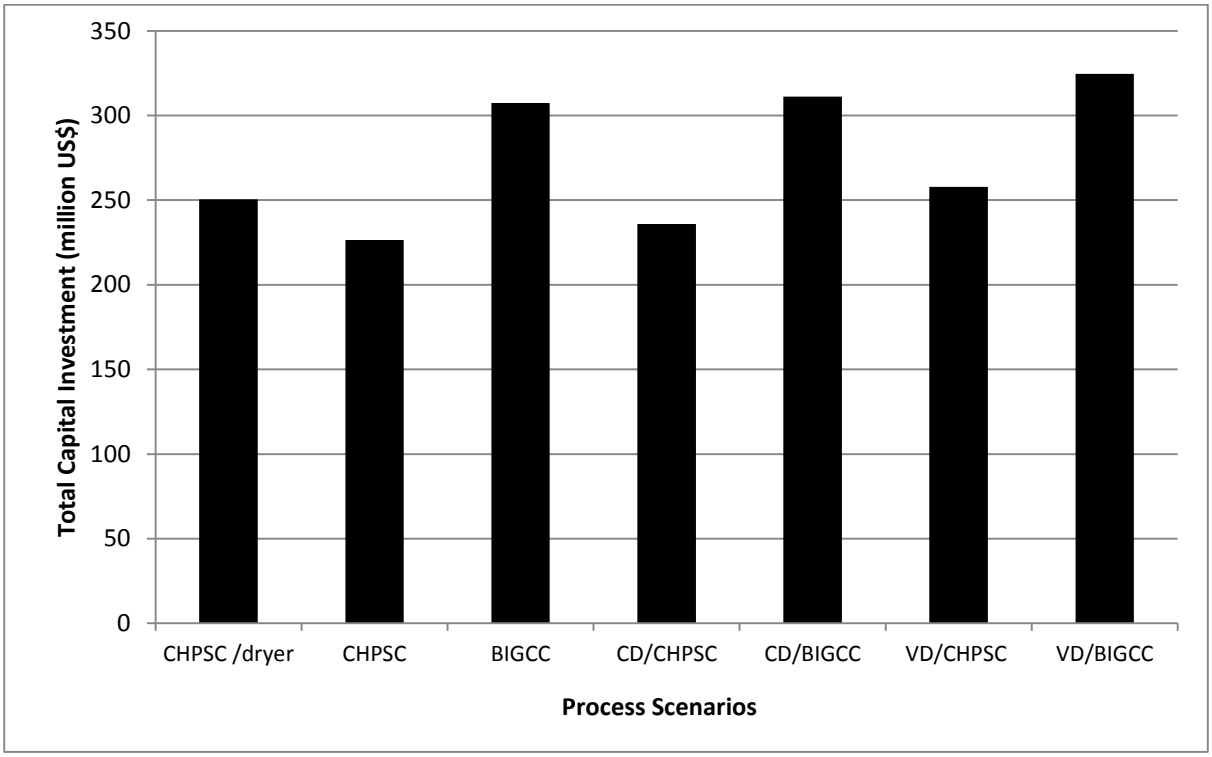


Figure 9: Total capital investment for simulated scenarios

The TCI of BIGCC-EE, which was based on a modern estimate[87], is 28.89% higher than the average TCI of CHPSC-EE. This difference is much less than those attained in previous comparative studies that based the BIGCC capital estimates on pioneer costs. The relative difference between BIGCC and the CHPSC technologies in Dornburg *et al*.[99] and

Bridgwater *et al*.[12] was about 50% and 77%, respectively. The difference in the comparison by Bridgewater *et al*. [12] had been exceptionally large, since the scale on which the comparison was based was a 20 MWe. Trends shown by Bridgewater *et al*[12]. and Dornburg *et al*. [99] have indicated that the difference gets smaller as the scale increases.

With regards to exclusive electricity production, it is shown (Figure 10) that the lowest IRRs were attained by the CHPSC-EE scenario, both inclusive and exclusive of the biomass dehydration prior to combustion. The IRRs obtained for the combustion scenarios did not differ significantly from each other, and on average were 22.38% (±0.98%) and 35.20% (±0.97%) at the minimum and maximum premiums on electricity, respectively. In either case, the higher value was obtained when no dryer was considered. Thus, the energy efficiency gained by employing a biomass dryer was not economically justified, due to the increased capital expenditure. The IRR attained by the BIGCC-EE is 7% and 6% higher than those attained by the CHPSC-EE scenario, when the minimum and maximum premiums on electricity were considered, respectively. In previous studies where the capital estimates of the BIGCC technology were based on pioneer quotes, the profitability of CHPSC technology was generally higher[12, 99]. As the capital estimate of the BIGCC technology in this study was based on a modern estimate, it shows that BIGCC-EE became more favorable, which had also been demonstrated by Searcy and Flynn[15].

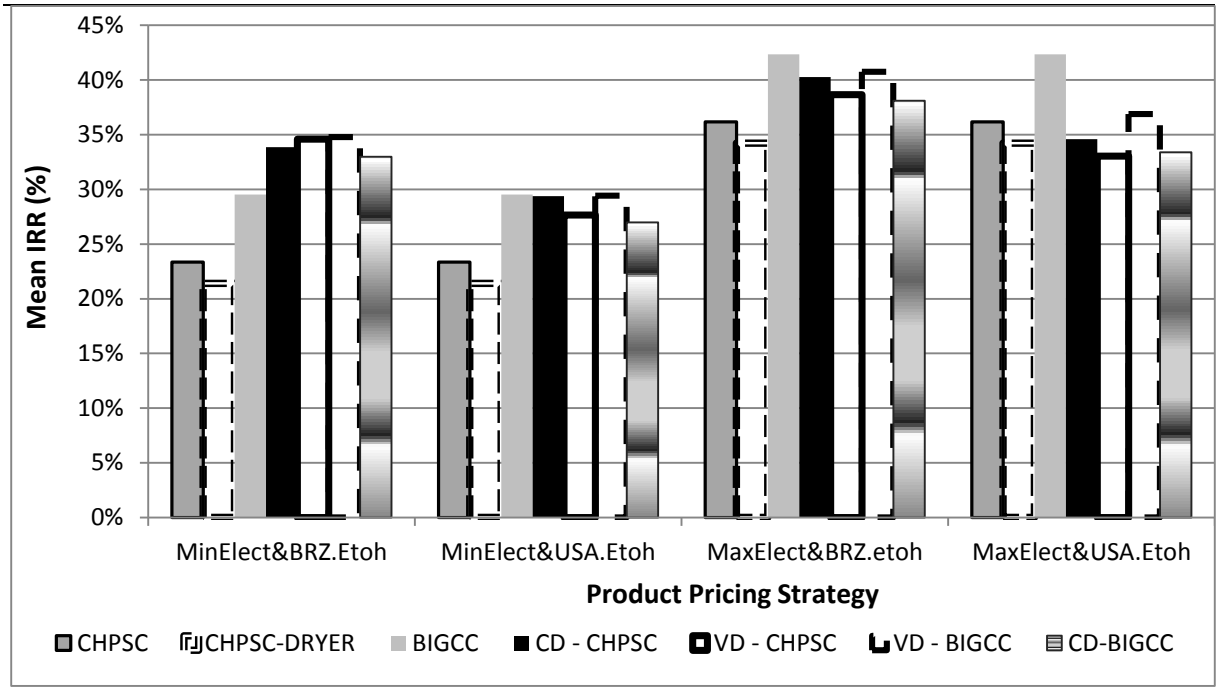


Figure 10: Comparison of processes profitability at varies strategies. "Mean IRR" refers to the average of the IRRs determined from each iteration of the Financial Risk Simulation.

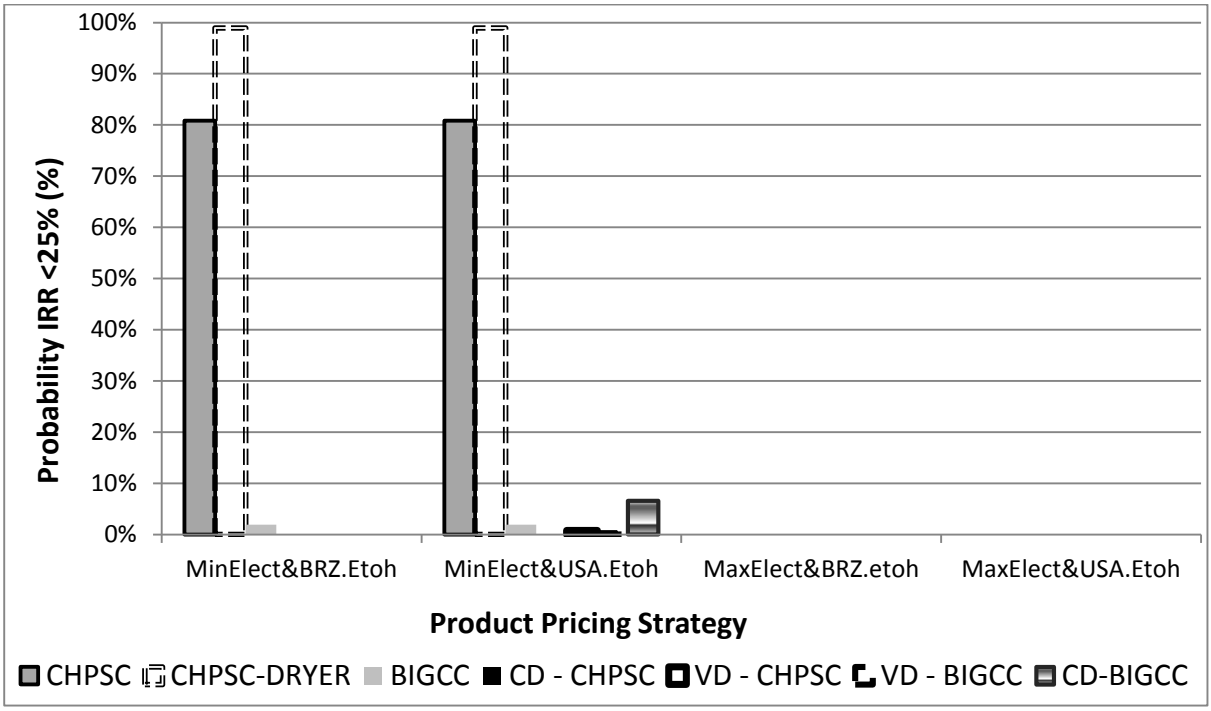


Figure 11: Evaluation of financial risk at varies pricing strategies. The value on the vertical axis describes the probability to which the IRRs simulated for each scenario will fall below a standard value of 25% for the IRR.

It was calculated that on average, the ethanol prices projected from Brazilian data were 47% greater than those based on US data, and therefore the overall minimum pricing strategy was the minimum electricity premium for electricity with US-based ethanol prices. At this pricing scenario, the highest profitability of the ethanol scenarios was attained by the VD/BIGCC. The economic feasibility of integrating BIGCC technology as the heat and power system of ethanol coproduction is advantageous over the CHPSC technology as the profitability of the VD/BIGCC was higher than the VD/CHPSC. This result was expected since the BIGCC-EE was more profitable than the CHPSC-EE when the exclusive electricity scenarios were compared due to the larger surplus of electricity. With regards to the implementation of VD, the IRR of the VD/CHPSC scenario was 1.05% lower than that of the CD/CHPSC, whereas the IRR of the VD/BIGCC was 1.48% higher than the CD/BIGCC. Thus, VD was not justified by the additional capital costs when integrated with CHPSC technology, but was more profitable when integrated with BIGCC technology. Due to the high amount of electricity that was needed for heating purposes in the CD/BIGCC scenario, the IRRs was lower than the VD/BIGCC, even though the capital expenditure was less.

When the maximum electricity premium was considered, the IRR of the BIGCC-EE was 1.59% higher than the most profitable ethanol scenario (VD/BIGCC) obtained with the higher (Brazilian) ethanol prices. Under the lower (US) ethanol pricing, the BIGCC-EE was 5.44% higher than the VD/BIGCC scenario (still the most profitable of the ethanol scenarios). Regarding the maximum electrical premium however, the IRRs shown in Figure 10 for exclusive electricity scenarios are well in excess of the standard IRR of 17% that is imposed by the National Energy Regulator of South Africa (NERSA) for independent power producers (IPPs)[100]. In order to diversify the renewable energy contribution of the South African

electricity supply (for example, from solar or wind), the prices paid to IPPs are regulated by NERSA to maintain an IRR of 17%, in order to promote equal investment opportunity in the various forms of renewable electricity[100]. Thus, as both the BIGCC-EE and CHPSC-EE are shown to meet this target at the minimum electricity premium, a higher price for electricity generated in the sugar mills would not be allowed.

With regards to assessing the scenarios from a financial risk perspective (Figure 11), the maximum occurrence at which the IRR can be less than 25% (which is known to attract the interests of private investors[36, 101]) was a probability of 20%. This qualification of 20% is an extension of a general criterion applied for the maximum probability of the net present value (NPV) being less than zero[102]. At the optimistic pricing scenarios, where high premiums on electricity are considered, all scenarios would be attractive for private investment (Figure 11) when the IRRs are evaluated against the IRR standard of 25%. An evaluation at the minimum pricing scenario showed that all ethanol coproduction scenarios qualified for private investment, since the risks associated with an unfavorable return for private investment were less than 1%, respectively. The maximum risks were attached to exclusive electricity production involving combustion, as the probabilities of the IRR falling below the standard of 25% were above 80.82% for the CHPSC-EE without drying and 98.96% with drying.

The status of the high risk imposed by the exclusive electricity scenarios to private investment would not improve due to restrictions imposed by NERSA on IPPs in respect of the standard IRR of 17%. However, sensitivity in the ethanol prices could allow for private investment that is virtually risk free when coproduction of ethanol is considered, as shown when ethanol prices are projected from the Brazilian data. Under that circumstance, the

risks of an unfeasible return for a private investor for all the ethanol scenarios are acceptable, even when the minimum premium for electricity is considered.

2.3 COMPARISON OF THE PRESENT STUDY WITH SIMILAR STUDIES IN PUBLISHED LITERATURE

Since the CHPSC-EE scenario was modelled on the flow sheet of Nsaful *et al*.[42], the results of this scenario was validated with the technical and economic results of the scenario using combustion and 82 bar steam cycle, in that study. The export efficiency calculated based on the electrical export of 86.02 kW per ton of cane amounts to 12.70%, which is lower than the export efficiency of 15.44% reported for the CHPSC-EE of this study. The export efficiency of this study is higher because the electricity generation was supplemented with sugarcane trash, which improved the amount of electricity available for export. The IRR reported for the process modelled by Nsaful *et al*. [42] was 29%, when a bagasse and electricity price of 56 US$/dry ton (data from 2010) and 0.248 U$ per kWhr are considered respectively. Under these conditions, the model in this study yielded an IRR of 41.82%. The optimistic outcome arose because the supplementation by trash improved the export electricity to 170.01 kW per ton of cane processed. Furthermore, the incorporation of trash, which costs just 30% of the bagasse price, reduces the average specific cost paid for biomass in the model of this study to 41.53 U$/dry ton (data from 2010).

The BIGCC-EE scenario was compared with the results of Craig and Mann[51], who conducted a techno-economic study of various options for a BIGCC power plant fueled by wood. Options explored included various gasification scenarios, such as pressurized versus near-atmospheric conditions, and direct versus indirect heating. Since this plant was an autonomous facility, the energy demands of the sugar mill were discarded in order to

remodel the BIGCC-EE scenario as an autonomous facility, so that the results could be comparable. The net electrical efficiency of the autonomous BIGCC-EE was 34.2%, which compared well with the value of 37.9% obtained by Craig and Mann[51]. The efficiency of Craig and Mann[51] is expected to be higher because the combined steam cycle of the pilot plant operated at the much higher pressure of 100 bar, which was a more efficient system for the steam cycle than the steam cycle in this study, which operated at a steam pressure of 60 bar. Thus a greater contribution was expected from the steam cycle section in that study[42]. Furthermore, Craig and Mann[51] assumed an efficient design of the gasifier that assured complete conversion of the biomass, whereas this study considered a conservative case where only 90 to 95% of the biomass was converted.

The minimum electricity price (MEP) determined by Craig and Mann[51] was 0.07 US$ per kWhr on a currency base of 1996, which is equivalent to a 2012 price of 0.132 US$ per kWhr. This was attained under the economic constraints of a biomass price of 78.67 US$ per dry ton (US$/d-ton) and an IRR of 10%. With such constrains, the exclusive BIGCC-EE of this study was shown to obtain a MEP of 0.10 US$ per kW/hr. The discrepancy then arises from the maturity of the capital cost estimates, as Craig and Mann [46] used very early stage estimates of BIGCC systems (1990), which was 51.97% more than the modern estimate (2008) used in the BIGCC scenarios of this study.

The results of the CD/CHPSC was compared to the feasibility assessment of an integrated ethanol facility conducted by Macrelli *et al*.[11], where the cellulose fractions of bagasse and trash residues were considered for second generation ethanol production. The net export efficiency of the integrated component, based on the export of electricity and lignocellulosic ethanol generated, was 35.2%, which is significantly higher than the

efficiency of 25.57% determined for the CD/CHPSC. This arose because Macrelli *et al*. [11] considered the cellulose fraction for ethanol production, which constitutes 35 to 40% of the considered biomass, as opposed to hemicellulose which only constitutes 20 to 24% of the considered biomass (see Table 2). Thus, a greater fraction of the biomass was efficiently used for the production of the energetic product.

The MESP (Minimum Ethanol Selling Price) that was determined for the lignocellulosic ethanol by Macrelli *et al*. [11] was 0.97 US$ per litre, under the economic constraints of a sugarcane trash price of 26 US$ per dry ton and an IRR of 10%. This MESP included a penalty of 0.12 US$ per litre for the reduction of export electricity when compared to electricity exports of an autonomous first generation facility and an enzyme cost of 0.38 US$ per litre. Thus, the MESP was adjusted to 0.47 US$ per litre by disregarding the penalty and enzyme cost, for a consistent comparison with this study. Under the economic constraints in the study of Macrelli *et al*. [11], the CD/CHPSC obtained a MESP of 0.43 US$ per litre, which compares well with the adjusted MESP of Macrelli *et al.* [11]. This comparison also shows that although a process converting cellulose to ethanol is more energy efficient, it is less economically viable due to the major cost associated with the enzymes needed to hydrolyse cellulose.

2.4 SENSITIVITY ANALYSIS

Figure 12 and Figure 13 show the economic sensitivity of the economic parameters to certain parameters that were deemed to have an uncertainty in their specification. The sensitivity was carried out with the pricing strategy that considered the minimum selling prices of electricity and ethanol. The coproduction scenarios with the highest profitability

were the VD/BIGCC and the CD/CHPSC, which were also the best indications of advanced and immediate technologies available, respectively. Thus, these scenarios were subjected to sensitivity analysis. Since the CD/BIGCC and VD/CHPSC were not as technically and economically viable, they were not included in the sensitivity analysis.

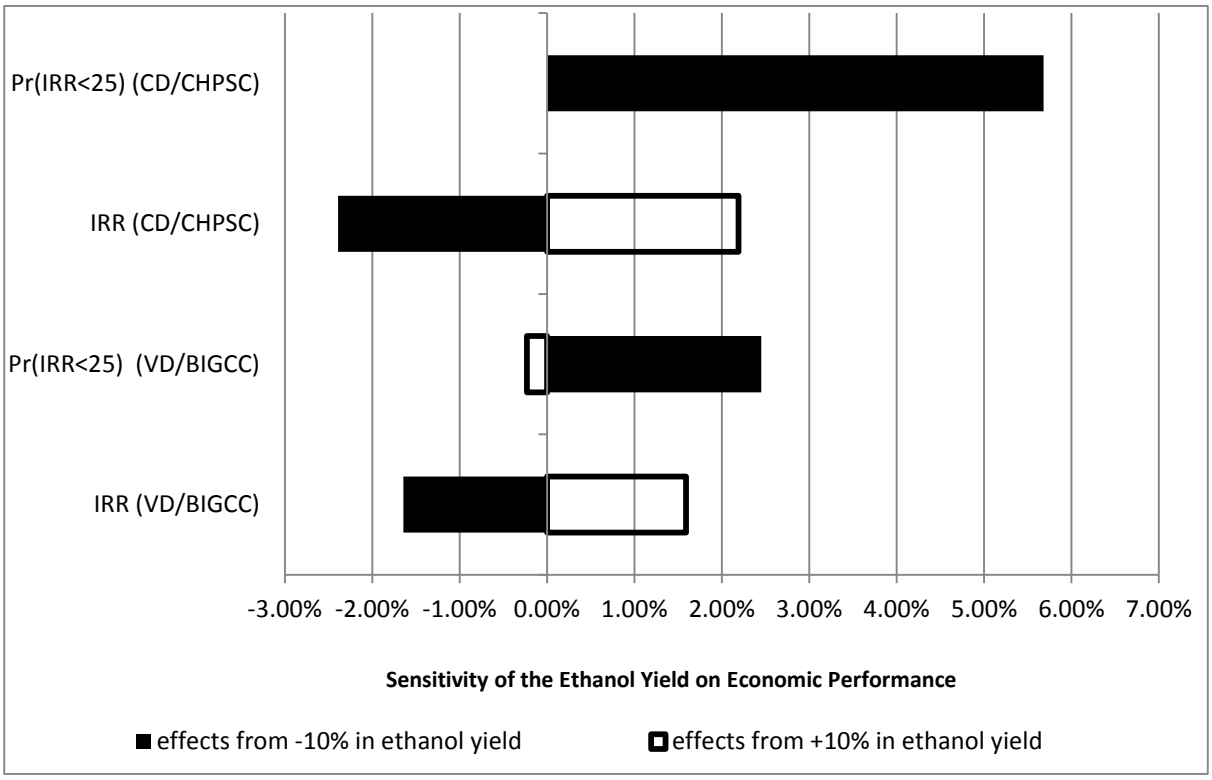


Figure 12: Sensitivity of the ethanol yield on the VD/BIGCC and CD/CHPSC scenarios.

With regards to the sensitivity of the overall ethanol output on profitability (Figure 12), a yield improvement of 10% generally increased the measured IRRs by 1.89%, which improved the IRR of the most optimal ethanol scenarios to 31.29 ± 0.29%. Alternatively, a yield that worsened by 10% reduced the IRRs by 2.02% on average to 27.38 ± 0.39%. The most important observation here is that a reduced yield had only increased the risk of the IRR receding below 25% by a margin of 5.68% at most (for the CD/CHPSC). Thus, the most economically viable ethanol scenarios remained desirable for investment from the private sector when sub-optimally performing technology was considered.

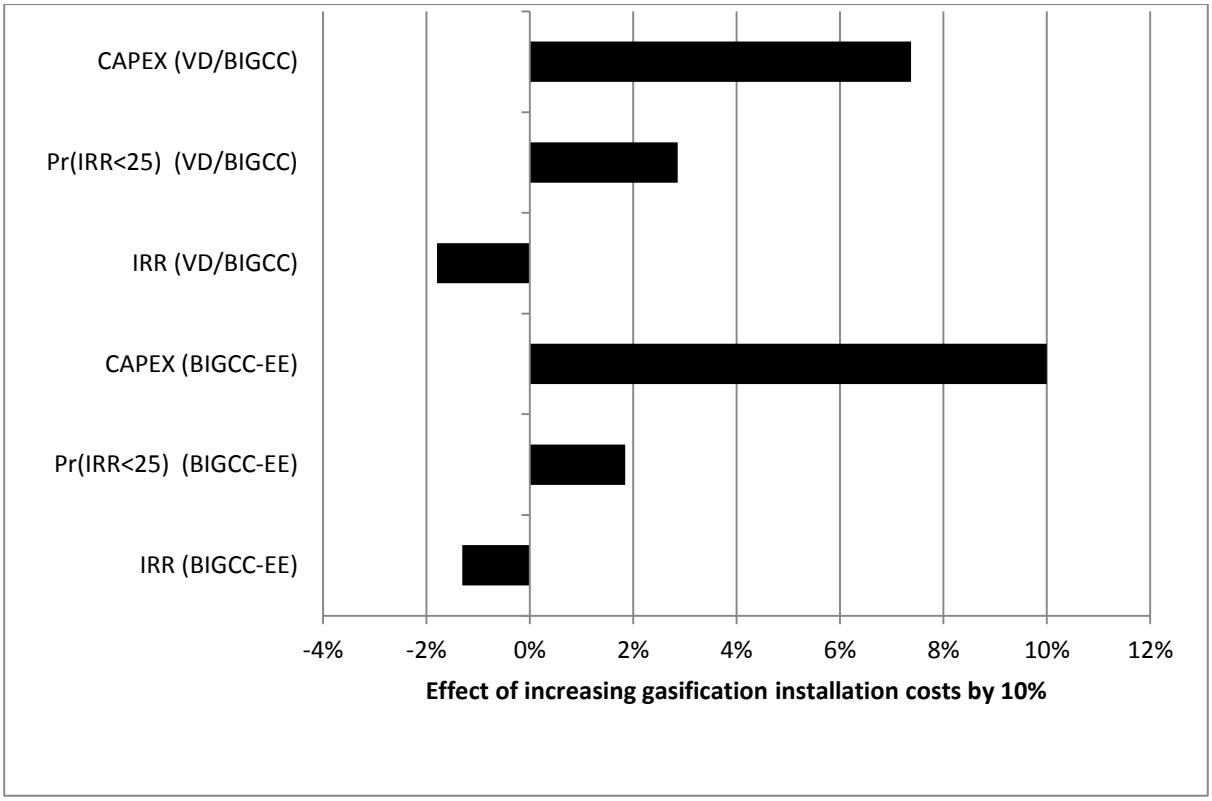


Figure 13: Effect of pessimistic installed estimate of gasification costs on the BIGCC-EE and VD/BIGCC scenarios. IRR – Rate of Return; Pr(IRR<25) – probability of IRR falling below 25%; CAPEX – Capital Expenditure

An increased estimate for the BIGCC installed costs of 10% (Figure 13) had increased the CAPEX for the BIGCC-EE by 10% and the VD/BIGCC by 7.35%. However, since the VD/BIGCC had the highest CAPEX originally, the effect of an increased installed cost was most prominent on this scenario since its IRR was reduced by a further extent than that of the BIGCC-EE. Given a reduction in the IRR of the BIGCC-EE of 1.31%, it is still far more viable than the CHPSC-EE scenario. Regarding the risk around private investment, the VD/BIGCC is still a viable option, as the probability of the IRR receding 25% was only 3.10%.

3 Conclusions

Ethanol coproduction with electricity generation has been shown to have greater exporting energy efficiency than exclusive electricity generation. This was demonstrated in

the context where the status of the electricity generation technologies is advanced, but where the technological status of ethanol production is at a conservative level, considering the modest conversion of sugars to ethanol using the detoxified hydrolysates. If a minimum pricing scenario on the ethanol and electricity products is considered, ethanol coproduction with electricity generation is considerably more profitable than CHPSC power plants, but on par with BIGCC power plants . The advantage of ethanol coproduction would become more pronounced as fermentation technology develops and matures as expected, and it would also become attractive for private investment. If the fermentation of hemicellulose hydrolysates (though successful on a bench-scale) can demonstrate that a pilot-scale conversion of at least 82.5% sugar to ethanol can be attained, it will confirm the technology proposed.

While a high premium on electricity would promote exclusive electricity production when ethanol prices are at a minimum, it is not likely that these premiums on electricity would be attained under the current regulations for renewable electricity in South Africa. The reason is because even at lower premiums, the IRR of the BIGCC-EE was 30%, whereas the prices of electricity for IPPs are regulated to allow for a maximum IRR of 17%.

The study showed that at the current scale, additional capital investments for more energy efficient technology is only justified when it effects a significant improvement in energy efficiency, as shown when BIGCC technology is used instead of the direct combustion in the ethanol coproduction schemes. Furthermore, it was found that when a more energy efficient technology only effected a minor improvement in energy efficiency, such as VD applied in the ethanol coproduction process or biomass dehydration in a combustion process, the economic returns did not justify the capital investment. There would be

situations however, where the energy intensity of the process would demand the implementation of such measures, either to reduce process steam demand or improve steam generation to a feasible operating range.

4 Abbreviations

BIGCC, Biomass Integrated Gasification and Combined Cycle; BOP, Balance of Plant; BRZ, Brazil; CD, Conventional Distillation; CEST, Condensing Extraction Steam Turbine; CFB, Circulating Fluidized Bed Reactor; CHPSC, Combustion with High Pressure Steam Cycle; DAH, Dilute Acid Hydrolysis; EE, Exclusive Electricity Production; E_{net}, Net Export Electricity; F, Ethanol Fuel; HRSG, Heat Recovery Steam Generator; IRR, Internal Rate of Return; KEI, Key Economic Indicator; n, net export efficiency; NPV, Net Present Value; NREL, National Renewable Energy Laboratory; PPA, Pinch Point Analysis; PPI, Producers Purchase Index; SA, South Africa; STEX, Steam Explosion; TCI, Total Capital Investment; *Technical Related;* USA, United States of America; VD, Vacuum distillation.

5 Competing interests

The authors declare that they have no competing interests.

6 Acknowledgements

The authors would like to thank Chair of Energy Research at Stellenbosch University, funded by the Department of Science and Technology, for providing financial assistance.

7 References

1. Mbohwa C, Fukuda S: **Electricity from bagasse in Zimbabwe**. *Biomass Bioenerg* 2003, **25**:197-207.

2. Dias MOS, Cunha MP, Jesus CDF, Rocha GJM, Geraldo J, Pradella C, Rossell CEV, Maciel R, Bonomi A: **Second generation ethanol in Brazil : Can it compete with electricity production ?** *Bioresour Technol* 2011, **102**:8964-8971.

3. Peacock S: **Process Design for Optimum Energy Efficiency**. *Tongaat Hullet Sugar* 2008.

4. Venkatesh KS, Roy AS: **Development and Installation of High Pressure Boilers for Co-Generation Plant in Sugar Industries**. *Smart Grid and Renewable Energy* 2010, **1**:51-53.

5. Ensinas AV, Nebra SA, Lozano MA, Serra LM: **Analysis of process steam demand reduction and electricity generation in sugar and ethanol production from sugarcane**. *Energy Conversion and Management* 2007, **48**:2978-2987.

6. Botha T, Von Blottnitz H: **A comparison of the environmental benefits of bagasse-derived electricity and fuel ethanol on a life-cycle basis**. *Energ Policy* 2006, **34**:2654–2661.

7. Dias MOS, Junqueira TL, Cavalett O, Cunha MP, Jesus CDF, Rossell CEV, Maciel R, Bonomi A: **Integrated versus stand-alone second generation ethanol production from sugarcane bagasse and trash**. *Bioresour Technol* 2012, **103**:152-161.

8. Huang H-jiang, Ramaswamy S, Al-dajani W, Tschirner U, Cairncross RA: **Effect of biomass species and plant size on cellulosic ethanol : A comparative process and economic analysis**. *Biomass Bioenerg* 2009, **33**:234-246.

9. Ogden J., Hochgreb S, Hylton M: **Steam economy and cogeneration in cane factories**. *International Sugar Journal* 1990, **92**.

10. Moor B: *Modern Sugar Equipment Assisting Cogeneration*. 2008:1-13.

11. Macrelli S, Mogensen J, Zacchi G: **Techno-economic evaluation of 2 nd generation bioethanol production from sugar cane bagasse and leaves integrated with the sugar-based ethanol process**. *Biotechnol Biofuel* 2012, **5**:22.

12. Bridgwater AV, Toft AJ, Brammer JG: **A techno-economic comparison of power production by biomass fast pyrolysis with gasification and combustion**. *Renew Sustain Energ Rev* 2002, **6**:181-248.

13. Caputo AC, Palumbo M, Ã PMP, Scacchia F: **Economics of biomass energy utilization in combustion and gasification plants : effects of logistic variables**. *Biomass Bioenerg* 2005, **28**:35-51.

14. Wang L, Weller CL, Jones DD, Hanna MA: **Contemporary issues in thermal gasification of biomass and its application to electricity and fuel production**. *Biomass Bioenerg* 2008, **32**:573-581.

15. Searcy E, Flynn P: **The Impact of Biomass Availability and Processing Coston Optimum Size and Processing Technology selection**. *Applied Biochemistry and Biotechnology* 2009, **154**:271-286.

16. Uddin SN, Barreto L: **Biomass-fired cogeneration systems with CO 2 capture and storage**. *Renewable Energy* 2007, **32**:1006-1019.

17. Faaij AP.: **Modern biomass conversion technologies**. *Mitigation and Adaptation Strategies for Global Change* 2006, **11**:343-375.

18. Kazi FK, Fortman JA, Anex RP, Hsu DD, Aden A, Dutta A, Kothandaraman G: **Techno-economic comparison of process technologies for biochemical ethanol production from corn stover q**. *Fuel* 2010, **89**:S20-S28.

19. Canilha L, Santos VT., Rocha GJ., Almeida e Silva J., Giulietti M, Silva S., Felipe MG., Milagres AMF, Carvalho W: **A study on the pretreatment of a sugarcane bagasse sample with dilute sulfuric acid**. *Journal of Industrial Microbiology and Biotechnology* 2011.

20. Purchase BBS, Walford SN, Waugh EJ: **AN UPDATE ON PROGRESS IN THE PRODUCTION OF ETHANOL FROM BAGASSE**. *Proceedings a/The SouthAfrican Sugar Technologists' Association - June 1986* 1986(June):33-36.

21. Treasure T, Gonzalez R, Venditti R, Pu Y, Jameel H, Kelley S, Prestemon J: **Co-production of electricity and ethanol , process economics of value prior combustion**. *Energy Conversion and Management* 2012, **62**:141-153.

22. Gnansounou E, Dauriat A, Wyman CE: **Refining sweet sorghum to ethanol and sugar : economic trade-offs in the context of North China**. *Biorefining* 2005, **96**:985-1002.

23. Gírio FM, Fonseca C, Carvalheiro F, Duarte LC, Marques S, Bogel-Lukasik R: **Hemicelluloses for fuel ethanol : A review**. *Bioresour Technol* 2010, **101**:4775-4800.

24. Kurian J., Minu A., Banerji A, Kishore VV.: **Bioconversion of hemicellulose hydrolysate of sweet sorghum bagasse to ethanol by using Pichia Stipitis NCIM 3497 and Debaryomyces Hansenii SP**. *Bioresources* 2010, **5**:2404-2416.

25. Nigam JN: **Ethanol production from wheat straw hemicellulose hydrolysate by Pichia stipitis**. *Journal of Biotechnology* 2001, **87**:17-27.

26. Rudolf A, Baudel H, Zacchi G: **Simultaneous Saccharification and Fermentation of Steam-Pretreated Bagasse Using Saccharomyces cerevisiae TMB3400 and Pichia stipitis CBS6054**. *Biotechnology and Bioengineering* 2008, **99**:783-790.

27. Humbird D, Davis R, Tao L, Kinchin C, Hsu D, Aden A, Schoen P, Lukas J, Olthof B, Worley M, D. Sexton and DD: **Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol**. *National Renewable Energy Laboratory* 2011(May).

28. Aden A, Ruth M, Ibsen K, Jechura J, Neeves K, Sheehan J, Wallace B, Montague L, Slayton A, Lukas J: **Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis for Corn Stover Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehyd**. *National Renewable Energy Laboratory* 2002(June).

29. Dias MOS, Modesto M, Ensinas AV, Nebra SA, Maciel R, Rossell CEV: **Improving bioethanol production from sugarcane : evaluation of distillation , thermal integration and cogeneration systems**. *Energy* 2011, **36**:3691-3703.

30. Grisales R, Cardona CA, Sanchez O., Guterrez L.: **HEAT INTEGRATION OF FERMENTATION AND RECOVERY STEPS FOR FUEL ETHANOL PRODUCTION FROM LIGNOCELLULOSIC**. *4th Mercosur Congress on Process Systems Engineering* 2005.

31. Kemp I.: **Pinch Analysis and Process Integration: A User Guide on Process Integration for the Efficient Use of Energy, Second Edition**. *Elsevier* 2007.

32. March L: *Introduction to Pinch*. Linnhoff March LTD; 1998.

33. Sue D-chern, Chuang C-chin: **Engineering design and exergy analyses for combustion gas turbine based power generation system**. *Energy* 2004, **29**:1183-1205.

34. Richardson JW, Herbst BK, Outlaw JL, Anderson DP, Klose SL, Gill II RC: *Risk Assessment in Economic Feasibility Analysis: The Case of Ethanol Production in Texas*. 2006.

35. Richardson JW, Lemmer WJ, Outlaw JL: **Bio-ethanol Production from Wheat in the Winter Rainfall Region of South Africa : A Quantitative Risk Analysis**. *Int Food Argibus Manag Rev* 2007, **10**:181-204.

36. Amigun B, Petrie D, Görgens J: **Economic risk assessment of advanced process technologies for bioethanol production in South Africa : Monte Carlo analysis**. *Renewable Energy* 2011, **36**:3178-3186.

37. Petersen A: **COMPARISONS OF THE TECHNICAL, FINANCIAL RISK AND LIFE CYCLE ASSESSMENTS OF VARIOUS PROCESSING OPTIONS OF SUGARCANE BAGASSE TO BIOFUELS IN SOUTH AFRICA**. University of Stellenbosch; 2012.

38. Wienese A, Purchase BS: **RENEWABLE ENERGY : AN OPPORTUNITY FOR THE SOUTH AFRICAN SUGAR INDUSTRY ?** In *Proceedings: The SouthAfrican Sugar Technologists' Association*. *Volume 78*; .

39. VAN DER WESTHUIZEN WA: **A TECHNO-ECONOMIC EVALUATION OF INTEGRATING FIRST AND SECOND GENERATION BIOETHANOL PRODUCTION FROM SUGARCANE IN SUB-SAHARAN AFRICA**. Stellenbosch University; 2012.

40. **South Afrcan Sugar Mills** [www.huletts.co.za/ops/south_africa/mills/felixton.asp]

41. Seabra JEA, Tao L, Chum HL, Macedo IC: **A techno-economic evaluation of the effects of centralized cellulosic ethanol and co-products refinery options with sugarcane mill clustering**. *Biomass Bioenerg* 2010, **34**:1065-1078.

42. Nsaful F, Görgens JF, Knoetze JH: **Comparison of combustion and pyrolysis for energy generation in a sugarcane mill**. *Energy Conversion and Management* 2013, **74**:524-534.

43. Leibbrandt NH: **Techno-Economics Study for Sugarcane Bagasse to Liquid Biofuels in South Africa: A Comparison between Biological and Thermochemical Process Routes**. *PhD Dissertation Department of Process Engineering University of Stellenbosch, University of Stellenbosch* 2010.

44. Diedericks D, Rensburg EV, Görgens JF: **Fractionation of Sugarcane Bagasse Using a Combined Process of Dilute Acid and Ionic Liquid Treatments**. *Applied Biochemistry and Biotechnology* 2012, **167**:1921-1937.

45. Oliveira FMV, Pinheiro IO, Souto-maior AM, Martin C, Gonçalves AR, Rocha GJM: **Industrial-scale steam explosion pretreatment of sugarcane straw for enzymatic hydrolysis of cellulose for production of second generation ethanol and value-added products**. *Bioresour Technol* 2013, **130**:168-173.

46. Mendes AGP: **Dust explosions**. *Proceedings: The South African Sugar Technologists' Association* 1999, **74**:282-288.

47. Department of Tourism and Air Quality .: *AQA Implementation: Listed Activities and Minimum Emission Standards*. 2008:Draft schedule for section 21Air Quality Act, Rev.

48. Nsaful F: **PROCESS MODELLING OF SUGAR MILL BIOMASS TO ENERGY CONVERSION PROCESSES AND ENERGY INTEGRATION OF PYROLYSIS**. Stellenbosch University; 2012.

49. Kreutz TG, Larson ED, Liu G, Williams RH: **Fischer-Tropsch Fuels from Coal and Biomass**. *25th Annual International Pittsburgh Coal Conference* 2008(August).

50. Mann MK, Spath SL: **Life Cycle Assessment of a Biomass Gasification Combined-Cycle System**. *National Renewable Energy Laboratory* 1997.

51. Craig KR, Mann MK: **Cost and Performance Analysis of Biomass-Based Integrated Gasification Combined-Cycle (BIGCC) Power Systems Cost and Performance Analysis of Biomass-Based Integrated Gasification Combined-Cycle (BIGCC) Power Systems**. *National Renewable Energy Laboratory* 1996(October).

52. Li XT, Grace JR, Lim CJ, Watkinson AP, Chen HP, Kim JR: **Biomass gasification in a circulating uidized bed**. *Biomass Bioenerg* 2004, **26**:171-193.

53. Rodrigues M, Walter A, Faaij AP.: **Performance evaluation of atmospheric biomass integrated gasifier combined cycle systems under different strategies for the use of low calorific gases**. *Energy Conversion and Management* 2007, **48**:1289-1301.

54. Fagbenle RL, Oguaka ABC, Olakoyejo OT: **A thermodynamic analysis of a biogas-fired integrated gasification steam injected gas turbine (BIG / STIG) plant**. *Applied Thermal Engineering* 2007, **27**:2220-2225.

55. Lugo-Leyte R, Zamora-Mata JM, M. Toledo-Vela´zquez, Salazar-pereyra M, Torres-aldaco A: **Methodology to determine the appropriate amount of excess air for the operation of a gas turbine in a wet environment**. *Energy* 2010, **35**:550-555.

56. Polyzakis AL, Koroneos C, Xydis G: **Optimum gas turbine cycle for combined cycle power plant**. *Energy Conversion and Management* 2008, **49**:551-563.

57. Ree RV, Oudhuis AB., Faaij A, Curvers APW.: *Modelling of a Biomass Integrated Gasifier Combined Cylce (BIG/CC) Sysrtem with the Flowsheet Simulation Programme Aspen Plus*. 1995.

58. Leibbrandt NH, Knoetze JH, Gorgens JF: **Comparing biological and thermochemical processing of sugarcane bagasse : An energy balance perspective**. *Biomass Bioenerg* 2011, **35**:2117-2126.

59. Gunarathne DS, Chmielewski JK, Yang W: *High Temperature Air / Steam Gasification of Steam Exploded Biomass*. 2013:1-14.

60. Aguilar R, Ramırez J., Garrote G, Vazquez M: **Kinetic study of the acid hydrolysis of sugar cane bagasse**. *Journal of Food Engineering* 2002, **55**:309-318.

61. Tricket R: **Utilisation of Bagasse for the Production of C5 and C6 Sugars**. University of Natal; 1982.

62. Lavarack BP, Gri GJ, Rodman D: **The acid hydrolysis of sugarcane bagasse hemicellulose to produce xylose , arabinose , glucose and other products**. *Biomass Bioenerg* 2002, **23**:367-380.

63. Carrasco C, Baudel HM, Sendelius J, Modig T, Galbe M, Zacchi G, Liden G: **SO2 catalyzed steam pretreatment and fermentation of enzymatically hydrolyzed sugarcane bagasse**. *Enzyme and Microbial Technology* 2010, **46**:64-73.

64. Ferreira-leitão V, Perrone CC, Rodrigues J, Paula A, Franke M, Macrelli S, Zacchi G: **An approach to the utilisation of CO 2 as impregnating agent in steam pretreatment of sugar cane bagasse and leaves for ethanol production**. *Biotechnol Biofuel* 2010, **3**.

65. Laser M, Schulman D, Allen SG, Lichwa J, Antal MJ, Lynd LR: **A comparison of liquid hot water and steam pretreatments of sugar cane bagasse for bioconversion to ethanol**. *Bioresour Technol* 2002, **81**:33-44.

66. Rocha GJM, Martín C, Vinícius FN, Gómez EO, Gonçalves AR: **Mass balance of pilot-scale pretreatment of sugarcane bagasse by steam explosion followed by alkaline delignification**. *Bioresour Technol* 2012, **111**:447-452.

67. Preez JC, Driessel BV, Prior BA: **Applied Microbiology Biotechnology Ethanol tolerance of Pichia stipitis and Candida shehatae strains in fed-batch cultures at controlled low dissolved oxygen levels**. *Applied Microbiology and Biotechnology* 1989, **30**:53-58.

68. Shevchenko SM, Chang K, Robinson J, Saddler JN: **Optimization of monosaccharide recovery by post-hydrolysis of the water-soluble hemicellulose component after steam explosion of softwood chips**. *Bioresour Technol* 2000, **72**:207-211.

69. Martin C, Galbe M, Nilvebrant N, Jonsson L: **Comparison of the Fermentability of Enzymatic Hydrolyzates of Sugarcane Bagasse Pretreated by Steam Explosion**. *Applied and Environmental Microbiology* 2002, **98-100**:699-716.

70. Nilverbrant N, Persson P, Reimann A, De Sousa F, Gorton L, Jonsson J: **Limits for Alkaline Detoxification of Dilute-Acid Lignocellulose Hydrolysates**. *Applied Biochemistry and Biotechnology* 2003, **105-108**:615-628.

71. Nigam JN: **Ethanol production from hardwood spent sulfite liquor using an adapted strain of Pichia stipitis**. *Journal of Biotechnology* 2001, **26**:145-150.

72. Alriksson B, Horvath I, Sjode A, Nilverbrant N, Jonsson L.: **Ammonium Hydroxide Detoxification of Spruce Acid Hydrolysates**. *Applied Biochemistry and Biotechnology* 2005, **121-124**:911-922.

73. Mcmillan JDJ: **Progress on Advanced Liquid Biofuels in the USA Biofuels**. In *International Symposium on Alchohol Fuels*; 2013.

74. Tantirungkij M, Izuishi T, Seki T, Yoshida T: **Applied Microbiology Biotechnoiogy Fed-batch fermentation of xylose by a fast-growing mutant of xylose-assimilating recombinant Saccharomyces cerevisiae**. *Applied Microbiology and Biotechnology* 1994, **8**:8-12.

75. Mcaloon A, Taylor F, Yee W, Regional E, Ibsen K, Wooley R, Biotechnology N: **Determining the Cost of Producing Ethanol from Corn Starch and Lignocellulosic Feedstocks Determining the Cost of Producing Ethanol from Corn Starch and Lignocellulosic**. *National Renewable Energy Laboratory* 2000(October).

76. Aspen Technology Inc: **Aspen Plus®, Aspen Icarus®**. 2008.

77. Aboyade A.: **CO GASIFICATION OF COAL AND BIOMASS : IMPACT ON CONDENSATE AND SYNGAS PRODUCTION**. *PhD Dissertation Department of Process Engineering University of Stellenbosch* 2012.

78. Chen C, Jin Y-qi, Yan J-hua, Chi Y: **Simulation of municipal solid waste gasification for syngas production in fixed bed reactors ***. *Journal of Zhejiang University-* 2010, **11**:619-628.

79. IChemE: **Pinch Point Analysis Spreadsheet**. 2006.

80. Peters and Timmerhaus: **Analysis of Cost Estmation Profitability, Alternative Investments and Replacements Optimum Design and Design Strategy**. In *Plant Design and Economics for Chemical Engineers,*. 5th Editio. McGraw Hill.; 1997.

81. Richardson JW, Klose SL, Gray AW: **An Applied Procedure for Estimating and Simulating Multivariate Empirical (MVE) Probability Distributions In Farm-Level Risk Assessment and Policy Analysis**. *Journal of Agricultural and Applied Economics,* 2000, **2**(August):299-315.

82. Richardson JW, Schumann K, Feldman P: **Simeter - Simulation & Econometrics To Analyze Risk**. 2008.

83. Bailey D: **Issues Analysis of Retrofitting Once-Through Cooled Plants with Closed-Cycle Cooling**. *Electric Power Research Institute (USA)* 2007.

84. Ridgway S.: **Projected Capital Costs of a Mist Lift OTEC Power Plant**. *The American Society of Mechanical Engineers* 1984.

85. Al-Riyami BA, Klimes J, Perry S: **Heat Integration reftrofit analysis of a heat exchanger network of a fluid catalytic cracking plant**. *Applied Thermal Engineering* 2001, **21**:1449-1487.

86. Rhodes JS, Keith DW: **Engineering economic analysis of biomass IGCC with carbon capture and storage**. *Biomass Bioenerg* 2005, **29**:440-450.

87. U S Environmental Protection Agency: *Biomass Combined Heat and Power Catalog of Technologies*. 2007(September).

88. **Eskom Tariffs and Charges** [www.eskom.co.za/content]

89. **CEPEA** [http://www.cepea.esalq.usp.br/xls/SaaofmensalUS.xls]

90. **Official Website** [http://www.neo.ne.gov/statshtml/66.html]

91. **Ethanol Prices** [www.card.iastate.edu]

92. **Producer Purchases Index** [www.statsa.gov.za/keyindicators/ppi]

93. **Reserve Bank, Historical Exchange and Interest Rates** [http://www.resbank.co.za/Research/Rates/Pages/SelectedHistoricalExchangeAndInterestRates.aspx]

94. Department of Minerals and Energy: **Biofuels Industrial Strategy of the Republic of South Africa**. 2007.

95. Eberhard A: **Grid-connected rewable energy in South Africa**. In *Presentation at the IFC,Washington 2013*; 2013.

96. Pellegrini LF, Junior S de O, Burbano JC: **Supercritical steam cycles and biomass integrated gasification combined cycles for sugarcane mills**. *Energy* 2010, **35**:1172-1180.

97. SAPIA: *Annual Report*. 2012.

98. **Generating Electricity** [http://www.eskom.co.za/c/article/208/generating-electricity/]

99. Dornburg V, Faaij AP.: **E ciency and economy of wood-ÿred biomass energy systems in relation to scale regarding heat and power generation using combustion and gasiÿcation technologies**. *Biomass Bioenerg* 2001, **21**:91-108.

100. NERSA: **NERSA Consultation Paper Review of Renewable Energy Feed - In Tariffs**. 2011(March).

101. Justice S: **Private Financing of Renewable Energy – A guide for policy makers,**. *UNEP* 2009.

102. Hacura A, Jadamus-Hacura M, Kocot A: **Risk analysis in investment appraisal based on the Monte Carlo simulation technique**. *THE EUROPEAN PHYSICAL JOURNAL* 2001, **B20**:551-553.

Chapter 5: Integration of Bioethanol Production in a the Paper and Pulp Industry

This chapter has been published in the journal "Biotechnology for Biofuels", volume 7, Issue 169 and can be downloaded at http://www.biotechnologyforbiofuels.com/content/7/1/169. It has been reproduced in this dissertation as is with the permission of the BioMed publication house.

Title of Article: "Techno-economics of integrating bioethanol production from spent sulfite liquor for reduction of greenhouse gas emissions from sulfite pulping mills"

Contribution of this Chapter

In this paper, flow-sheet analysis was used to develop a feasible process for bioethanol production from spent sulphite liquor (SSL) (digestion liquor) containing mostly pentose sugars. This process was integrated into a sulphite pulping process Based on the chemical characterisation of SSL, flow-sheets for simulations on ethanol production were constructed by combining design elements found in literature with plant data and guidelines given by experts from the Saiccor mill.

In relation to the overall of this dissertation, it was found that integrated bioethanol production from SSL at the Sulphite mill would not attract private investment if the performance is based on an SSL with conservative characteristics (i.e. a sample that had most diluted content of sugars). However, a performance based on SSL feed with characteristics that is representative of a time-averaged sample (implying that the sugar content increases) will attract private investment. In relation to the general objectives to do extended flow sheet analysis, it was shown that it is essential in terms of the greenhouse gas reduction potential of the biofuel life cycle that the supplementary fuel to satisfy the overall energy balances be from renewable sources, else the life cycle will accrue

global warming emissions. This occurred because the SSL substrate had a low concentration of sugars.

Authors' contributions

AMP is the primary author and investigator of the research in this paper. KH is the internal reviewer and brought the quality of English up to standard. JFG is the study group leader and approved the paper as a formal submission from the research group. All authors read and approved the final manuscript.

Petersen et al. Biotechnology for Biofuels 2014, 7:169
http://www.biotechnologyforbiofuels.com/content/7/1/169

Biotechnology for Biofuels

RESEARCH ARTICLE Open Access

Techno-economics of integrating bioethanol production from spent sulfite liquor for reduction of greenhouse gas emissions from sulfite pulping mills

Abdul M Petersen, Kate Haigh and Johann F Görgens*

Abstract

Background: Flow sheet options for integrating ethanol production from spent sulfite liquor (SSL) into the acid-based sulfite pulping process at the Sappi Saiccor mill (Umkomaas, South Africa) were investigated, including options for generation of thermal and electrical energy from onsite bio-wastes, such as bark. Processes were simulated with Aspen Plus® for mass- and energy-balances, followed by an estimation of the economic viability and environmental impacts. Various concentration levels of the total dissolved solids in magnesium oxide-based SSL, which currently fuels a recovery boiler, prior to fermentation was considered, together with return of the fermentation residues (distillation bottoms) to the recovery boiler after ethanol separation. The generation of renewable thermal and electrical energy from onsite bio-wastes were also included in the energy balance of the combined pulping-ethanol process, in order to partially replace coal consumption. The bio-energy supplementations included the combustion of bark for heat and electricity generation and the bio-digestion of the calcium oxide SSL to produce methane as additional energy source.

Results: Ethanol production from SSL at the highest substrate concentration was the most economically feasible when coal was used for process energy. However this solution did not provide any savings in greenhouse gas (GHG) emissions for the concentration-fermentation-distillation process. Maximizing the use of renewable energy sources to partially replace coal consumption yielded a satisfactory economic performance, with a minimum ethanol selling price of 0.83 US$/l , and a drastic reduction in the overall greenhouse gas emissions for the entire facility.

Conclusion: High substrate concentrations and conventional distillation should be used when considering integrating ethanol production at sulfite pulping mills. Bio-wastes generated onsite should be utilized at their maximum potential for energy generation in order to maximize the GHG emissions reduction.

Introduction

Ethanol production can be integrated with a paper and pulp facility, however, the energy balance needs to be optimized due to the energy-intensive nature of both processes [1-3]. Energy-efficient integration of bioethanol production into processes such as the magnesium oxide (MgO) acid sulfite pulping process provides opportunities for the co-production of bio-energy products with existing pulp products. In sulfite pulping processes, such as those used by the Sappi Saiccor mill in Umkomaas, South Africa, the energy requirements for the pulping process are provided by concentrating the spent sulfite liquor (SSL), which contains dissolved lignocellulosic components, such as lignin derivatives and hemicellulose sugars, and feeding the resulting syrup to a recovery boiler [2]. The energy generated from the combustion of SSL is often not sufficient to satisfy the energy demands of the mill itself, and an additional fuel source, such as bark, biomass residues or coal, is needed [2,4]. If the sugar components in SSL are converted to ethanol, the calorific input to the recovery boiler would reduce, increasing the reliance on a supplemental fuel source, which in the case of Saiccor is coal. This demand for supplemental energy

* Correspondence: jgorgens@sun.ac.za
Department of Process Engineering, University of Stellenbosch, Cnr Banghoek and Joubert Street, 7600 Stellenbosch, South Africa

will be compounded with the energy demands of an integrated ethanol facility.

The energy demands of existing ethanol production from molasses or syrup come primarily from the ethanol separation and purification section of the process [5]. The energy demand of such distillation processes is directly related to the concentration of ethanol in the fermentation beer that serves as distillation feedstock [1,6]. In turn, this concentration is dependent on the concentration of fermentable sugars in the feed substrate (the SSL), and the efficiency of sugar conversion to ethanol during fermentation [6]. The fermentation of SSL poses challenges in both aspects, as the sugar concentrations of SSL (between 2 and 3% (w/w)) are lower than required [6-8]. In addition, the presence of toxins, such as organic acids and furans, create an inhibitory environment for the yeasts, which reduces fermentative activity [6,7,9]. Sugars represent 25 to 30% of the total dissolved solids (TDS), which implies that SSL sugars cannot be concentrated to more than 50 to 60 g/l. At this point, the TDS of 30% will become inhibitory to fermentation due to osmotic stress and media viscosity [6,7,9], even for detoxified SSL. These limitations imply that the SSL fermentation products will typically contain 20 g/l of ethanol, which is significantly less than the minimum of 40 g/l required for energy- efficient distillation [10].

Nonetheless, the fermentation of SSL on a laboratory scale has shown considerable success, using both native xylose fermenting strains and genetically modified (GM) strains. Nigam [7] conducted fermentation experiments using *Pichia stipitis* on an SSL sample derived from hardwood via a calcium oxide (CaO) sulfite process, and was able to achieve an ethanol yield of 70% (of total sugars) at a dissolved solids content of 26%, resulting in a maximum ethanol concentration of 20.5 g/l. In order to achieve this performance the strain was adapted through prior growth in SSL that was treated with alkaline detoxification. Without prior adaption, a sugar-to-ethanol conversion of 10% was achieved. A recent attempt using mutants of *P. stipitis* for fermenting hardwood SSL was made by Bajwa *et al.* [11]. While all sugars were used, the results show that an excess amount of ethanol was metabolized, since the ethanol yields only ranged from 60 to 65%. Using a GM strain (*Saccharomyces cerevisiae* 256ST), Helle *et al.* [9] was able to obtain yields of 85% and 76% on MgO-based SSL samples derived from eucalyptus wood, having dissolved solid contents of 20% and 30%, respectively. This was without detoxification, and final ethanol concentrations of 16.5 g/l and 22.5 g/l were attained.

The energy integration of ethanol production into a sulfite pulp mill is challenging because of the energy demands of the ethanol process and the reduction of the energy content of the SSL available as the boiler fuel. The reliance of the combined pulping-ethanol process on supplementary fuel sources would thus be increased. Coal is presently the default source of supplementary heat and power at Sappi Saiccor due to installed coal-fed boilers (CFB). However, the use of fossil fuels would devalue the net greenhouse gas reductions (NGHGRs) associated with the production of ethanol as a fossil fuel replacement. A study has shown that the NGHGR of United States-produced corn-ethanol, powered by fossil fuels, was 47%, compared to 74% for Brazilian-produced sugarcane-ethanol because the sugarcane residues were used to provide energy and export electricity [12,13]. Biomass-to-energy (BTE) systems for combined heat and power (CHP) are typically less efficient than coal-based systems due to the lower calorific value of biomass [14]. Consequently, the economic viability of energy production from biomass has only been realized when the cost for obtaining the biomass is low [15]. Large amounts of forestry residues are generated at pulp mills at approximately 460 kg (bark, branches, tops and leaves) per ton of wood chips processed [16]. The use of bark for energy generation is an established strategy for supplementing the energy needs of pulping mills in the United States [4]. Another option for renewable energy to supplement the energy demands of the pulp mill is the biodigestion of organic-rich effluents for the production of biogas [17].

The present study investigated strategies for integrating ethanol production into an MgO sulfite pulping plant, to achieve both the intended NGHGRs and economic viability, based on the flow rates of, and samples shipped from the Sappi Saiccor mill as industrial representatives. The Sappi Saiccor mill is an acid sulfite pulping mill situated in Kwazulu-Natal, South Africa, which produces virgin cellulose pulp from wood, primarily *Eucalyptus globulus*. Furthermore, various CHP scenarios were combined with the various ethanol production processes, to obtain an economically viable and environmentally beneficial scenario. The study aims to represent a conservative case regarding ethanol production, by considering flow sheet inputs from the SSL samples that were received with the lowest sugar concentration. In this way, the energy demands will be overestimated and the ethanol production will be underestimated.

Various flow sheets were considered, with the objective being to minimize the combined energy requirements of SSL concentration and ethanol distillation. All the ethanol production scenarios assume the use of an industrial yeast strain with the same (or superior) capabilities of the GM strain *S. cerevisiae* 256ST used by Helle *et al.* [9], and substrate detoxification as a conservative design step. The distillation of the crude products to anhydrous ethanol will also consider variants, such as multi-effect and conventional distillation (CON), which pose advantages in steam and electricity use, respectively [18].

Results and discussion

Chemical analysis

The chemical analysis for the sugars, organic acids, furans, total phenolic compounds and the total polymeric compounds (TPC) present in the SSL are shown in Table 1. The organic acids and furans are important indicators of the inhibitory nature of the SSLs as fermentation feedstock, and compared well to the literature [7]. The acetic acid was present at 4.26 (0.47%) to 9.02 g/l (0.99%), while previous reports indicated 9.3 g/l [7] and 0.8% [8]. The furfural concentration was measured at 0.239 g/l, compared to 0.2 g/l [7,8] that was previously measured. The concentration of the total phenolic compounds at 125.5 mg/l was lower than that reported by Marques *et al.* [8].

The concentration of total sugars (glucose, xylose and arabinose) in the SSL was 20.49 g/l, which was lower than the measurements by Marques *et al.* [8] for the same stream from the Sappi Saiccor facility, and the previous measurement of 28.47 g/l from a previous shipment of samples (data not shown). Flow sheet analysis based on the measurements in Table 1 would thus represent a pessimistic estimation of the energy performance of an integrated ethanol facility, especially with regards to the concentration of ethanol in the fermentation beer.

Evaluation of process energy considerations and greenhouse gas emission characteristics

The technical information describing the ethanol scenarios (refer to Table 2 for a description of the scenario names), with supplemental energy supply to satisfy the net demands of the integrated pulping-ethanol process, are presented in Table 3. Equations 1 and 2 were used to calculate the equivalent values of the coal required to generate the steam and electricity demands for the base case scenarios; at an excess of what is currently required by the pulping facility. The greater value between the equivalent amounts of coal determined for electricity and thermal energy defined the coal requirement for the respective scenario. This is because coal supplied at the lower equivalent value would result in a deficient generation of the utility that required the higher coal demand. Regarding the amounts of steam and electricity generated by the BTE system, these are in excess of the demands of the ethanol production scheme, and would partially fulfil demands of the pulping facility and displace the equivalent amount of coal. In these energy scenarios, if the amount of coal displaced is greater than the lower of the equivalents of coal determined, this would result in a deficit in the supply of that utility corresponding to the lower equivalent. In those cases (i.e. the BTE augmented schemes), the limiting displacement of coal

Table 1 Results for chemical analysis of spent sulfite liquor samples (HPLC – high performance liquid chromatography; MgO – magnesium oxide; CaO – calcium oxide; SSL – spent sulphite liquor; HMF – hydroxyl-methyl-furfural; TPC – total polymeric compounds)

	Unit	MgO-SSL		CaO-SSL	
HPLC Measured		**Amount**	**Error**	**Amount**	**Error**
Furfural	g/l	0.29	0.01	0.23	0.01
HMF	mg/l	4.50	0.50	6.00	2.00
Formic Acid	g/l	0.81	0.08	2.21	0.04
Acetic Acid	g/l	4.26	0.35	9.02	0.15
Glucose	g/l	1.38	0.06	2.78	0.06
Xylose	g/l	18.25	1.16	27.68	0.45
Arabinose	g/l	0.86	0.07	1.18	0.01
Phenolics	mg/l	48.55	2.86	23.85	1.40
Solids	%	10.95	0.05	14.39%	0.10%
Ash	% of Solids	10.34	1.25	8.76%	0.00%
Elemental Composition					
Carbon	%	5.78	0.25	8.41%	0.29
Hydrogen	%	10.32	0.36	9.46%	0.34
Nitrogen	%	0.59	0.16	0.23%	Maximum[a]
Sulphur	%	1.45	0.13	2.64%	Maximum[a]
Oxygen	%	81.86	Difference	81.18%	Difference
Calculated TPC	%	8.99%		13.70%	

[a]The elemental analyser measures organic sulphur and nitrogen by the SO_2 and nitric oxides respectively, which are generated during combustion of the sample. The CaO ash generated during the combustion of Ca SSL absorbs acidic gasses [19], which then causes variability in the sulphur and nitrogen in this particular sample. Thus, the maximum value is reported as a conservative measure. Since the Ca SSL is only considered for biodigestion of the non-recalcitrant sugars, with no further processing, this result does not affect the outcomes of the simulations in any way.

Table 2 Summarized description of scenarios considered (TDS – total dissolved solids; CON- conventional distillation; ME – multi-effect distillation; BG – biodigestion; BTE- biomass to energy)

		Ethanol Process Alternative			
		20% TDS, Convention Distillation	20% TDS, Multi-effect Distillation	30% TDS, Convention Distillation	30% TDS, Multi-effect Distillation
Energy Generation Alternatives	Coal Fired	20-CON	20-ME	30-CON	30-ME
	Coal Fired with Biodigestion	20-CON-BG	20-ME-BG	30-CON-BG	30-ME-BG
	BTE	20-CON-BTE	20-ME-BTE	30-CON-BTE	30-ME-BTE
	BTE with Biodigestion	20-CON-BTE-BG	20-ME-BTE-BG	30-CON-BTE-BG	30-ME-BTE-BG

was defined by the lower value of the equivalent's values determined for steam and electricity.

The energy demands of the ethanol production processes were compared in terms of distillation (multi-effect under vacuum versus conventional) and sugar concentration in the SSL feed. The heat integration potential of multi-effect distillation (ME) resulted in a reduction in the steam demand of 42.41%, compared to the CON scenarios. However, the ME scenarios also required 70.10% more electricity than the conventional scenarios, due to the demands of the vacuum pump between the beer and rectifier columns. Overall, ME needed 55.78% more coal equivalents than the conventional scenarios, primarily due to the high thermal energy demands of steam-based electricity generation. Higher sugar concentrations in the SSL with 30% TDS reduced the electricity and steam demands by an average of 16.93% and 9.40%, respectively, due to lower volumes of fluid processed per unit of ethanol produced.

The results in Table 3 shows that the extent to which excess energy supply from the BTE augmented system could substitute the existing coal consumption was limited by the electrical demand, in case of ME, and steam demand for the CON scenarios. Displacement of existing coal utilization with surplus BTE energy supply was 17.40% higher for the multi-effect scenarios than for the CON scenarios. For the base cases however, where all of the energy requirements were met by coal combustion, the CON scenarios were advantageous over the ME, due to lower coal requirements. The difference is due to the boiler pressure used in each energy generation scheme, which impacts the electrical generation efficiency. The pressure ratio of the CFB and BTE steam cycles were 6.1 and 10.6, respectively, which resulted in a specific electricity generation of 0.092 MW and 0.125 MW per ton of steam generated, respectively. Thus, per ton of steam produced, the BTE system generated more electricity than the CFB system, thus favoring scenarios with higher electrical demands.

The NGHGR of the base case scenarios (driven by coal only) were all negative, which implied that integration of ethanol production into the pulp mill would worsen GHG emissions over the process life cycle, compared to the pulping-only processes.,. As the global warming potentials ((GWPs) the – NGHGR) are in accordance with the coal required for the various scenarios, the lowest GWP of 10,821.18 kg $CO_{2(eq)}$ was achieved by the 30-CON, while the highest GWP of 23,159.77 ton/hr $CO_{2(eq)}$ was attained by the 20% solids-multi-effect scenario (20-ME). While additional energy supplementation through biodigestion reduced the coal consumption for the base scenarios by 0.90 tons/hr (14.95%), the reduction in the GWP potentials were not enough affect a positive NGHGR. The NGHGR values of the BTE augmented schemes are all positive, indicating that the integrated ethanol-pulping facility significantly reduced GHG emissions of the process life cycle, compared to the pulping-only facility. As these ratios are in accordance with the coal displacement potentials, the best NGHGR of 23,579.43 tons/hr $CO_{2(eq)}$ was attained by the 30-ME-BTE scenario. When digestion is considered in conjunction with a BTE system, the coal displacements are typically improved by 0.96 tons/hr while the NGHGRs were improved by 14.90% on average.

Economic results

The total capital investment (TCI) of all scenarios considered is shown in Figure 1. The coal-only scenarios represented the lowest TCIs of the ethanol production processes, as the existing coal boiler will be used. The lowest capital investment of US$ 36,710,000 was for the 30-CON. This is due to the high sugar concentrations in the SSL feedstock resulting in a high ethanol concentration and thus lower volumetric throughputs and smaller equipment sizes. Furthermore, the equipment costs associated with the vacuum pump for ME is negated. Comparing the two distillation configurations shows that ME increased the TCI by 61.90%. Accordingly, the highest capital requirement was needed by the 20-ME scenario.

Comparing economic viability, as measured by the internal rate of return (IRR) (Figure 2), it is shown to be strongly related to capital investment, as the IRR of the 30-CON (base) was in just short of 25%, while that of the 20% solids-multi-effect scenario (20-ME) (base) was just about 1%. The economic viability is also related

Table 3 Analysis of effect of integration of ethanol production on energy characteristics (CON- conventional distillation; ME – multi-effect distillation; BTE- biomass to energy)

Scenarios	Ethanol Cogeneration				Current Recovery
	20%-ME	20%-CON	30%-ME	30%-CON	
Concentrated SSL Flow rate (tons/hr)	135.21		95.94		
Net Outputs					
Bioethanol Production (l/hr)	2,555.63	2,556.35	2,321.48	2,321.48	
Steam Utilities					
Gross Steam Generation (tons/hr)	124.35	125.11	124.23	124.50	135.54
Total Steam Demand (tons/hr)	52.77	73.77	53.68	63.70	45.17
Total Additional Steam Utility Required (tons/hr)	18.79	39.03	19.82	29.56	
Electricity Generation and Requirements					
Gross Electricity Generation (MW)	13.39	13.46	13.37	13.40	14.60
Power and/or Ethanol Utilities (MW)	5.27	2.80	4.13	2.19	0.41
Total Additional Electricity Utility Required	6.08	3.53	4.95	2.99	
Base Case - Coal Driven					
Coal for Steam Demand (tons/hr)	2.59	5.38	2.73	4.08	
Coal for Electricity Demand (tons/hr)	8.08	4.71	6.59	3.99	
Required Supply (tons/hr)	8.08	5.38	6.59	4.08	
Net Greenhouse Gas Reduction Potential (tons/hr)	−23,159.77	−15,129.65	−18,300.52	−10,821.18	
BTE Augmented Scenarios					
Steam Supply (tons/hr)	75.80	75.80	75.80	75.80	
Electricity Generation (MW)	10.57	10.57	10.57	10.57	
Displacement of Coal (tons/hr)	−5.97	−5.07	−7.46	−6.38	
Utility Causing Maximum Coal Displacement	Electricity	Steam	Electricity	Steam	
Net Greenhouse Gas Reduction Potential (tons/hr)	18,720.18	16,034.64	23,579.43	20,343.11	
Biodigestion - Coal Driven Scenarios					
Required Supply (tons/hr)	7.32	4.32	5.63	3.25	
Net Greenhouse Gas Reduction Potential (tons/hr)	−20,904.11	−11,951.92	−15,449.50	−8,350.75	
Biodigestion - BTE Augmented Scenarios					
Displacement of Coal (tons/hr)	−6.73	−6.14	−8.42	−7.44	
Net Greenhouse Gas Reduction Potential (tons/hr)	20,975.84	19,212.37	26,430.45	23,523.50	

to coal consumption, demonstrated by the increase in the IRR for scenarios with decreased coal consumption. Furthermore, it is shown that the higher yield of ethanol possible with a more diluted SSL substrate (i.e. dissolved solids at 20%) did not justify the additional capital and process costs compared to fermentation with 30% SSL.

The installation of a BTE system is shown to bear substantial capital costs, as shown by an increase of almost three-fold in the base capital costs of the 30-CON scenario when a BTE was installed. However, installation of a BTE for coal replacement generally increased the IRR of the combined ethanol-energy facility, thus justifying the additional capital costs. The BTE installation improved the economic viability of the 20-ME scenario the most, due to a lower increase capital requirement and substantial coal displacement, in contrast to intensive use of coal in the coal-only scenario.

The installation of biodigestion generally had a negative effect on the economic viability (in contrast to the installation of BTE) as shown by a decrease in the IRR. The IRR of the 20-ME scenario, however, increased by 2.17% due to biodigestion installation, because there was a minor effect on the overall capital requirements. The most severe was a decrease of 5.54% in the IRR for the 30-CON, due to the significant effect of capital requirements for biodigestion in this particular scenario. The combination of biodigestion with BTE augmented scenarios resulted in an average decrease of 1.83% in the IRR, compared to BTE augmented scenarios without biodigestion. Thus, inclusion of biodigestion is shown to have a negative effect on economic viability, since the savings it generates by

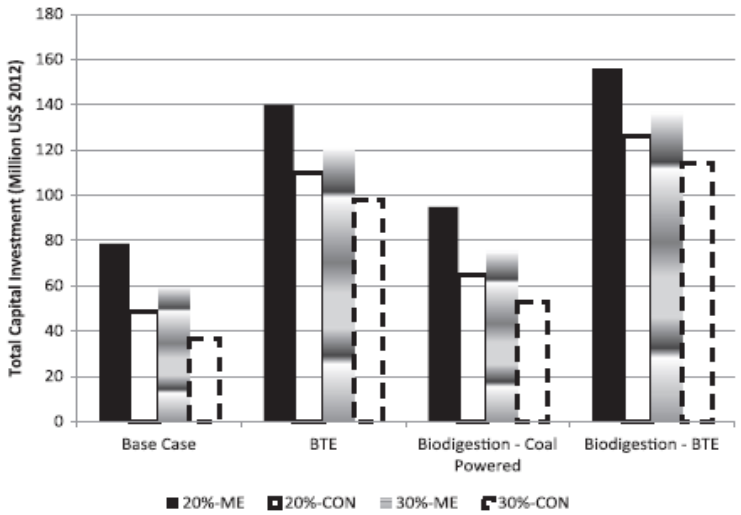


Figure 1 Total capital investment. (CON- conventional distillation; ME – multi-effect distillation; BTE- biomass to energy).

coal supply reductions are not enough to justify the capital expenditure.

In Figure 2, the relationship between the IRR and the NGHGR is shown for all the process scenarios considered. For the coal-fed scenarios, the minor improvement in life-cycle reduction of GHG emissions that biodigestion offered was not economically justifiable. In addition, the significant improvements in GHG reductions that the BTE augmentation afforded generally caused an improvement in the IRR as well, which implies that the overall costs of a BTE system are cheaper than coal. Of the BTE scenarios, the 30-ME-BTE scenario had the highest net GHG emission reductions, while the 30-CON scenario had the best economic viability, due to its lower TCI. This pattern was also observed when biodigestion was considered with BTE.

Analysis on plant scale and minimum ethanol selling price

A subsequent analysis was carried out on the effect of economies of ethanol production scale on the economic viability of the 30-CON-BTE-BG (BG-biodigestion) scenario. Again, citing the Sappi Saiccor facility as an example, the SSL throughput was doubled by assuming

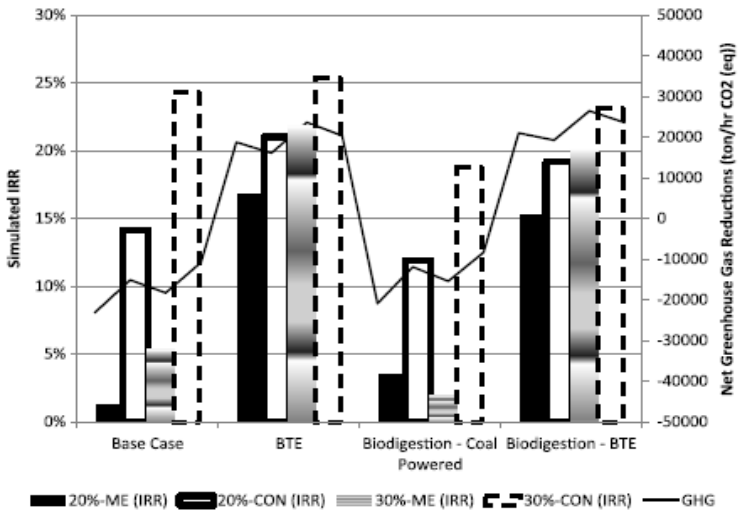


Figure 2 Simulated IRR of the various scenarios in relation to net GHG reductions. (CON- conventional distillation; ME – multi-effect distillation; BTE- biomass to energy).

that both of the MgO SSL streams would be directed to ethanol fermentation, instead of fermenting one of the streams. The 30-CON scenario with digestion was selected for this analysis because it offered the greatest potential for environmental benefits, though it was not attractive for private investment (IRR less than 25%). The impact of the increase of scale by a factor of two on the minimum ethanol selling price (MESP), coal displacement, NGHGRs and IRR was determined.

Doubling the rate of ethanol production resulted in an increase in electrical and thermal energy demands, which was met by the combination of biodigestion and BTE (Figure 3). The energy scheme was also capable of providing a surplus of energy to displace coal at a rate of 2.12 tons/hr, although it was less than coal displacement at the smaller scale. Doubling the ethanol production scale also reduced the NGHGR by 49.98% when compared to the smaller scale. The reduction in the NGHGR and coal displacement was because the scale of the BTE system remained static, while the demands of energetic utilities had increased significantly due to the increase in scale by a factor of two. Thus, the resulting IRR only improved by an absolute amount of 3.73%, (16.13% relative) ,which is a mild effect when compared to previous reports on the effect of economies of scale [20], where a scale-up of about two-fold in production capacity in an integrated ethanol plant resulted in about an 80% increase in economic viability.

The MESP required to produce an IRR of at least 25%, with an 80% probability of surpassing this benchmark, was determined for the smaller and larger production scale of the 30-CON scenario. The MESP of 0.82 US$/l for the smaller scale was unfavorable, relative to Brazil (0.67 US $/l) and the United States (0.61 US$/l), although it improved by 9.6% to 0.71 US$/l for the larger scale. In a South African context, the MESP of the small-scale production compares favorably with the preliminary price of 1.07 US$/l for first-generation ethanol determined in the South African Department of Energy biofuel strategy [21].

Sensitivity of the net greenhouse gas reductions potential, internal rate of return and the minimum ethanol selling price to initial substrate concentrations

Comparison of SSL-fermentation scenarios was based on a measured total sugar concentration of 20.49 g/l in SSL before concentration (Table 1), which was shown to be lower than the sugar concentration measured in samples of previous shipments. The impact of higher sugar concentrations in the SSL on the economic viability and environmental benefits (NGHGR) of the 30-CON-BTE-BG scenario was thus determined. The impact of the increase in sugar concentration of the ethanol production rate was determined for the IRR, MESP and NGHGR (Figure 4).

The increase of 39% in the sugars concentration in SSL significantly improved economic viability, as reflected in an increase of 7.86% in the IRR and reduction of the MESP by 27.83% - to a value of 0.58 US$/l. Operating the digesters in the sulfite pulping process at the highest solids (woodchips) loading would thus increase the sugar concentration in the SSL and subsequently benefit the associated ethanol process. At an expected average sugar concentration of 24.61 g/l in the SSL, an IRR of 27.03% can be achieved if the ethanol selling price based on average international prices of ethanol is assumed. Regarding the NGHGR, a marginal increase of 6.25% can be expected, due to the increased production of ethanol and the subsequent increase in displacement of gasoline.

Conclusion

The preferred scenario for integration of ethanol production from MgO-SSL into a sulfite mill was SSL with 30%

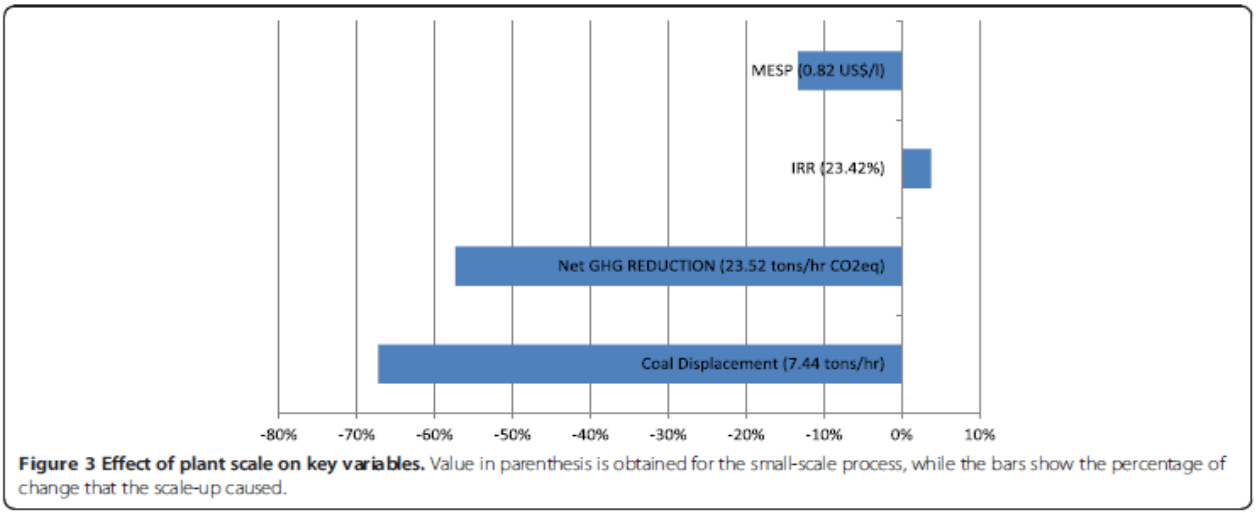


Figure 3 Effect of plant scale on key variables. Value in parenthesis is obtained for the small-scale process, while the bars show the percentage of change that the scale-up caused.

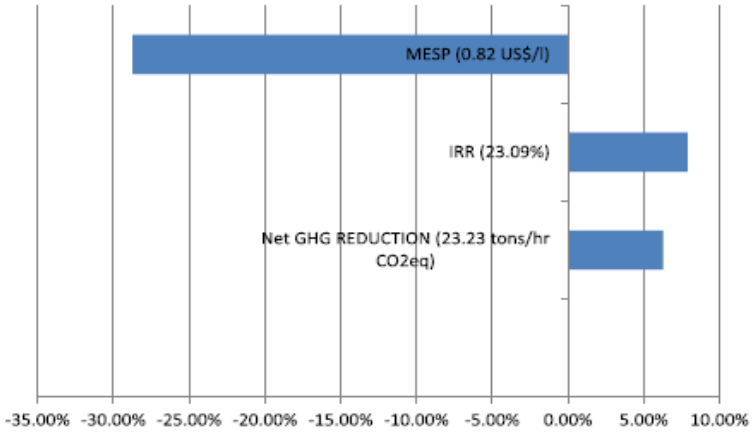


Figure 4 Effect of initial SSL sugar concentration on key variables. Value in parenthesis is resulted for the diluted feed, while the bars shows the percentage of change that the concentrated substrate caused.

TDS from the existing multi-effect concentrator as feedstock, and purifying the ethanol from the resulting fermentation broth using CON. The capital costs of this process was lowest when using coal to supply all of the energy demands of the integrated pulping-ethanol process, although there was an increase in greenhouse gas emissions. Maximum use of thermal and electrical energy generation from bark (combustion) and evaporator effluents (biodigestion) to replace coal consumption provided satisfactory economic viability and significant greenhouse gas reductions. In addition, the chemical oxygen demand (COD) of the effluent discharge was reduced. The effect of scaling the ethanol production by considering two MgO-SSL streams as fermentation substrates, instead of just one, had improved the IRR, but also reduced the NGHGR.

Through the rigorous methodology of flow sheet development, a scheme for integrating the production of ethanol, as well as thermal and electrical energy from biowastes, into a pulping mill was developed. Economically, the optimized flow sheet is highly competitive against first-generation ethanol in South Africa, even at a small production scale, and could compete with international ethanol prices at larger scales. Less conservative estimations than applied in the present investigation may further improve the IRR, or lower the MESP, of the resulting process.

In this study, it was assumed that the effects of the inorganic chemicals that are used to condition the SSL for fermentation on the recovery boiler would be significant and thus the costs associated with these effects were conservatively estimated. Thus, it is recommended that a detailed study be carried out to determine these effects, so that an energy efficient and cost effective means of mitigating the effects can be found if those effects are shown to be significant enough to intensify the operation of the recovery boiler system. These studies however, are likely to be carried out privately, as the knowledge of the exact operation of these systems is not in the open literature.

Methodology

Overview of the acid sulfite process

The pulping process begins by de-barking, then chipping wood-logs. The woodchips are mixed with water and pulping liquor, followed by pulping with SO_2 injection in the digesters, to solubilize lignin and hemicellulose sugars [22]. The crude pulp discharged from the digesters is washed with water in a counter-current vacuum filter system and the clean pulp is sent for chemical bleaching and mechanical pulping, while the wash-filtrate, referred to as SSL, is processed by concentration and combustion [22]. A brief schematic flow is provided in Figure 5.

The Sappi Saiccor facility has three acid sulfite lines, two of which are MgO-based (MgO1 and MgO2), and one that is CaO-based [22]. The SSL from the two MgO lines are concentrated in separate trains of evaporators to form boiler feed syrup for energy production and pulping chemicals recovery. Of the SSL from the CaO line, 70% is sold to an adjacent lignosulfonates processing facility, while the rest is discharged as an industrial effluent (personal communication with B. Chizwanza and C. Reddy). Thus, the MgO-SSL line is more appropriate as a substrate for ethanol production, while the effluent portion of the CaO-SSL is available as substrate for biodigestion. In the present study only one of the MgO-SSL streams is considered for ethanol production, while the processing of the second MgO-SSL line remains unaltered.

Materials and analysis

Samples of the SSLs were shipped from the Sappi Saiccor facility and analyzed for monomeric sugars,

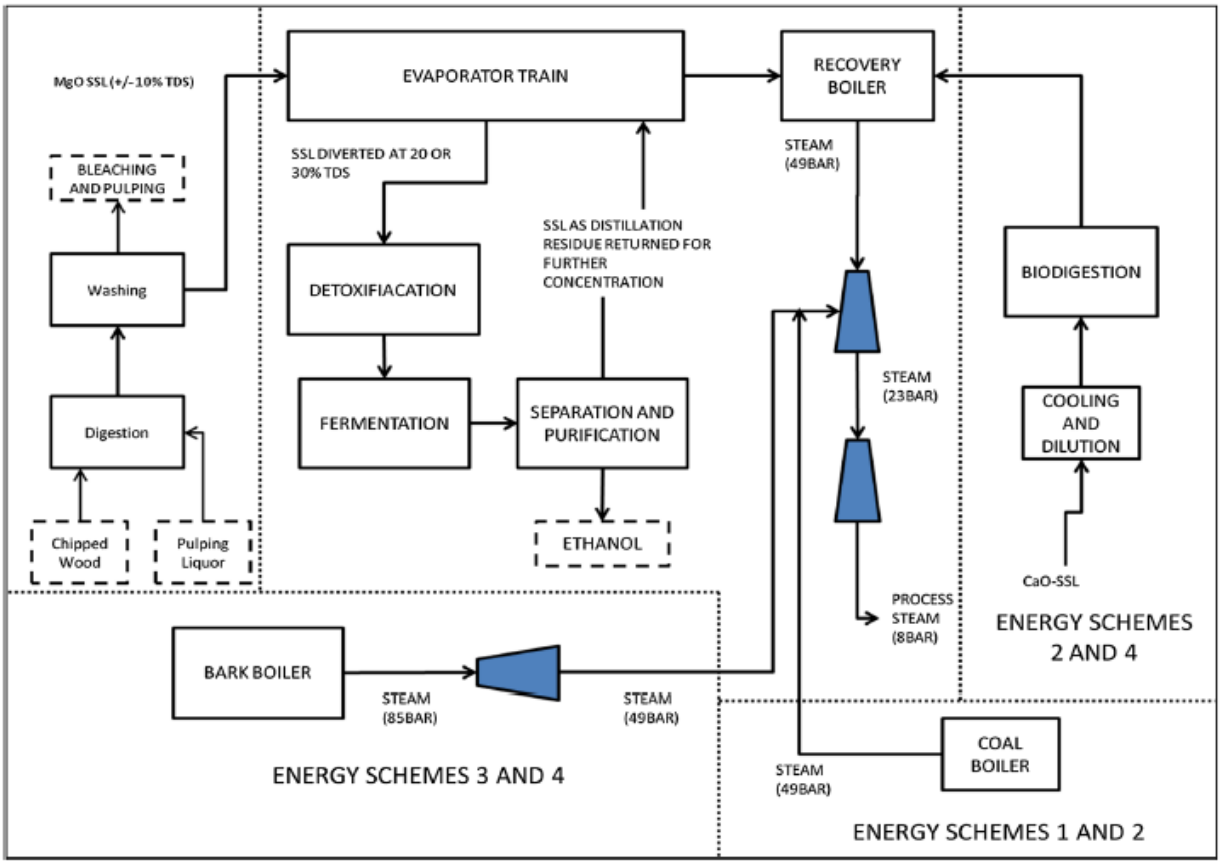


Figure 5 Schematic overview of the scenarios for ethanol integration and energy generation schemes. (TDS-total dissolved solids; MgO – magnesium oxide; CaO – calcium oxide; SSL – spent sulphite liquor)

organic acids, furans [7,8] and phenolic compounds [23] using high performance liquid chromatography (HPLC analysis), as previously used for acid hydrolysates [24,25]. In order to determine the TDS, the samples were dried at 110°C over a sufficient period for the samples to be bone dry. The dried samples were then combusted at 725°C in order to determine the ash content.

The elemental composition of the SSL was also analyzed using a LECO TrueSpec Micro elemental analyzer (LECO® Corporation, Worldwide) to determine the carbon, hydrogen, nitrogen and sulphur contents, with the oxygen content determined by difference. As the organic content of SSL typically comprises polymeric sugar/lignin compounds, extractives, monomeric sugars, organic acids and furans [8], the chemical formula and quantity of the TPC were determined as the difference between the total atomic make-up (shown by the elemental analysis) and the total portion of these elements found in the measured compounds.

Process development

Given the low concentration of sugars generally found in SSL, the liquor requires concentration prior to fermentation. In cited literature [6,7,9], the range of TDS concentration generally considered for fermentation is 20 to 30%, where the sugar concentrations would typically be in the range of 50 to 70 g/l. Thus, the ethanol plant would be integrated into the existing evaporation trains at a sulphite mill, by diverting the SSL syrup for ethanol feedstock from after the concentrating stage, where the TDS concentration is 20% or 30%. The process flow sheet for the various integration strategies is shown in Figure 5.

The first process step after concentration in the ethanol production process is detoxification. Detoxification with lime is deemed impractical on an industrial scale, due to the large quantities of gypsum created [6]. Instead, detoxification with soluble compounds, such as sodium hydroxide or ammonium hydroxide, are better alternatives to avoid these issues and both have previously been shown to be effective at improving fermentability [26]. The choice

depends mainly on the effect of these chemicals on the ANDRITZ chemical recovery system (recovery boiler) (ANDRITZ AG, Graz, Austria) that is presently operating at the Sappi Saiccor facility [27]. Detoxification with sodium hydroxide and sulfuric acid was selected, as the resulting sodium sulphate in the SSL residues after fermentation will have a minor impact on the existing system, since the ANDRITZ recovery scrubber (ANDRITZ AG, Graz, Austria) already has sections dealing with water-soluble ashes [27]. However, as a conservative measure to account for the associated costs, it will be assumed that the scrubber will be modified with a bag filter to capture the extra load of condensing alkali salts in order to avoid corrosion. The capital and maintenance costs of the bag filters will be taken from the National Renewable Energy Laboratory (NREL) [28,29] reports.

The detoxified SSL will be filtered to remove flocculants that might have formed during detoxification, before splitting about 3 to 4% of it to acclimatize the yeast to toxic environments during cell production. The fermentation performance of a robust recombinant strain of *S. cerevisiae*, reported to convert more than 80% of the pentose sugars in an untreated SSL sample to ethanol [9], was assumed for concentrated detoxified SSL. Specifically, conversions of 85% and 76% of the sugars were considered for the 20% and 30% substrates respectively [9], at cell concentrations of 3 to 5 g/l. Thus, the inclusion of detoxification is a conservative measure to assure high yields, as it had previously been shown that conversions without detoxification could be reduced by 60% [7]. With regards to the electrical energy needed to agitate the fermentation tanks, half of the specific rate of 11 MJ_e per ton of substrate that estimated from the NREL reports [28] for hydrolysis and fermentation was considered, as there were no hydrolysis reactors in this study. Heat removal is done with chilled water at 15-20°C provided by a chiller, which operates at a coefficient of performance of seven [30].

The beer from fermentation is first heated and flashed at 0.86 bar to remove the CO_2, which is sent to a knockout drum to recover ethanol, followed by ethanol recovery through scrubbing of the vapor from the knockout drum [31]. The liquid effluents from the flash vessel, knockout drum and scrubber are combined and further combined with the fermentation beer into the distillation train [31]. This train can be either conventional, where the beer stripper and rectifier columns are both atmospheric, or a multi-effect system where the beer stripper column is under vacuum, to allow the heat released by the rectifier condenser to effect the reboiler of the beer stripper [32,33]. In either case, the distillation system produces vapor phlegm that is 91% ethanol, which may be dehydrated with molecular sieves to an anhydrous quality of 99.7% ethanol [31], depending on market demand.

The syrup produced as the beer stripper bottoms is returned to the evaporation train for concentration of the remaining TDS content to 60%, and subsequent combination with the MgO SSL syrup not used for fermentation, as feed to the recovery boiler. The recovery boiler produces superheated steam at 49 bar pressure, which is sequentially expanded to 23 bar and 8 bar, to provide the required live steam in the plant. Heat recovery from the stack gasses from the boilers is currently sufficient to reduce the temperature of the stack gasses to 135°C. As further information about the energy recovery scheme was not available, it is assumed that the recommended energy recovery measures, such as an economizer after the boiler and an air pre-heater, are applied as components in recovering heat from the stack [2,4]. Further measures for recovery boiler operation, like minimizing the excess air fed to meet the environmental regulatory requirement of the oxygen content being 6% in the stack gas, are also assumed to apply [34].

Establishment of the reference case for the current utility usage

Estimations of industrial flow-rates of SSL citing the Sappi Saiccor facility are conservatively estimated to be 285 ton/hour for each of the three process lines (for MgO1, MgO2 or CaO). Only one of the MgO lines are considered for ethanol production, again giving a conservative economic estimate in terms of the economies of scale of ethanol production, and minimizing the impact of ethanol production on the overall pulping-ethanol energy balance. The reference case on which to base ethanol production scenarios is the current processing of SSL, which is concentration in a multi-effect system followed by energy and chemicals recovery in the recovery boiler. The data from Perin-Levasseur *et al.* [35] was used to simulate the six-effect evaporator for SSL concentration in Aspen Plus [36], (Aspen Technology, Inc, Massachusetts, United States of America (USA)) together with simulation of the recovery boiler. From these simulations, the following reference points for the existing MgO-SSL evaporator train and recovery boiler could be established: 1) the concentration of TDS of the streams leaving each evaporator, so that concentrated SSL streams with 20% TDS or 30% TDS could be withdrawn and compared in ethanol production scenarios; 2) the heat duty of each evaporator; 3) the amount of steam produced by the recovery boiler that is currently consumed by the mill and 4) the amount of electricity generated by the turbines, and that is consumed by equipment like the boiler feed pump and combustion air fans. The net available electricity from power generation is presently consumed by the mill.

Simulation of ethanol scenarios

The four ethanol scenarios were simulated as the combination of two possible TDS concentrations in the SSL feed

from the existing evaporator train, and two possible distillation schemes. For each scenario, the syrup is returned from the distillation section to the remaining stages of the evaporation trains, and then subsequently fed to the recovery boiler system. The necessary simulation of the pumping costs will all be accounted for in the simulation. Thus, from the simulation of ethanol scenarios in Aspen Plus [36] and the subsequent comparison with the values determined for the reference case, the sets of information attained and calculated are as follows: 1) the production rate of ethanol, chemical requirements and energy generation of the recovery boiler system from the syrup returned after distillation; 2) the minimum hot and cold utility duties calculated by recording the heating and cooling demands from the simulations and processing these through Pinch Point Analysis using the ICheme spreadsheet [37]; 3) the net steam and electrical utility requirements calculated as the difference in the increased utility demands of the integrated plant to the reference case, and the deficit in the utilities generated by the recovery boiler of the integrated facility, compared to the recovery boiler of the reference case.

Simulation of external energy generation schemes

The combined heat and power plants that provide energy to both the pulping and ethanol processes, using either biomass or coal, were simulated in Aspen Plus [36], according to the approach recommended by the Aspen Plus manual [38]. The chemical characteristics of two fuel types are presented in Table 4. The thermal energy recovery scheme from combustion (described in the process development section) for the recovery boiler is assumed to extend to the existing CFB boilers and the new BTE augmentation system proposed for supplementation of the process energy supply [39]. Figure 5 depicts how the flow of the energy streams from these systems is integrated into the overall systems of the various energy schemes.

Table 4 Chemical characteristics of bark and coal

Proximate Analysis %		
Material	**Coal [40]**	**Bark [41]**
Moisture	5.00	47.50
Fixed Carbon	55.40	6.60
Volatile Matter	27.00	41.50
Ash	12.60	4.40
Elemental Analysis (% Moisture Free)		
Hydrogen	4.42	5.52
Carbon	70.63	49.12
Nitrogen	1.79	0.38
Sulphur	0.72	0.04
Oxygen	9.18	36.56
Ash	13.26	8.38

The thermal and electrical utilities of the combined pulping-ethanol plant, in excess of what would be provided by the existing recovery boilers, was quantified in terms of the equivalent amount of coal required for the CFB boilers. Thus, the Aspen Plus model for coal-to-energy was simulated with a range of coal flow rates, using the sensitivity analysis feature. From the data generated, a set of linear equations that related the coal-fed versus steam and net electricity generation were produced, which was then used to determine the equivalent amount of coal needed for the utilities. Thus, the steam generated is determined by Equation 1 and net electricity generated is determined by Equation 2:

$$\text{STEAM} = 7.249 \times \text{COAL} + 0.008 \quad (1)$$

$$\text{ELECTRICITY} = 0.755 \times \text{COAL} - 0.021 \quad (2)$$

For the BTE system, a flow rate of 34 tons/hour of bark was considered, based on current supply from the digestion capacity of 8,000 tons of wood a day [22], and the rate of bark generation at 150 kg per ton of wood prepared [16]. In order to achieve a high electrical generation efficiency in the BTE system, this boiler will operate at a pressure of 85 bar [42]. This steam will be expanded in a back-pressure turbine to 49 bar so that it can be injected into the current steam expansion-extraction system.

Supplemental energy for the recovery boiler was also obtained by biodigestion of a portion of the CaO-SSL, presently disposed as effluent. The CaO-SSL was diluted with mild process wastewaters, to reduce the COD from a value of >170 to 79 g/l so that the stream would be suitable for biodigestion microbes [17]. The CaO-SSL was also cooled by means of a heat exchanger to a temperature of 40°C to ensure a temperature of about 35°C after dilution, which is optimal for microbe activity [17]. The microbes generate biogas by fermenting the non-recalcitrant components in an up-flow anaerobic sludge blanket (UASB) reactor which, for a typical SSL stream, reduces the COD by 20% [17]. The biogas is then used to supplement the fuel of the recovery boiler, since the recovery boilers at Sappi Saiccor have ports through which supplemental gas is fed.

Scenario development

The ethanol production scenarios could consider two substrate concentration levels (20% or 30%), which would either be combined with ME or CON distillation, and thus four ethanol production schemes (20-ME, 20-CON, 30-ME, 30-CON) are possible. The energy supply scheme for all the ethanol scenarios could either consider additional coal (base case), the BTE augmentation system, supplementation of biogas generated from CaO-SSL biodigestion or a combination of BTE augmentation and

supplementation of biogas. The coal-driven scenarios are described in their base form (for example, 30-CON), while the biodigestion- and BTE-driven scenarios have the description amended with BTE or BG (for example, 30-CON-BTE, or 30-CON-BG). With all renewable energy supplementation included, the descriptions are amended with BTE-BG (for example, 30-CON-BTE-BG).

Technical evaluation

The various ethanol scenarios were evaluated based on the amount of additional coal needed to drive the process. If a biomass boiler was considered, then the steam or electricity generated in excess of the demands of the ethanol integration was converted to an equivalent amount of coal that would be replaced. The effect of supplementing the recovery boiler with biogas generated from the biodigestion of the CaO-SSLon the overall energy balance, in terms of the amount of coal it replaces was also evaluated.

Net greenhouse gas reductions

Since this study involves renewable energy products from processes driven with fossil and renewable energy sources, the determination of the NGHGR is imperative. The NGHGR has been defined as the negative the GWP, that is, NGHGR = –GWP. Life-cycle assessment techniques adapted for process evaluations were applied to compare the GWP of each scenario [43-45]. The system boundary for the GWP determination included all of the affected sub-systems in the processes, which was begun with the diversion of the MgO-SSL from the evaporation train to ethanol production. Thus, it included the chemical manufacture and transport, coal mining and transport, ethanol production, utility generation and coal displacement. As this study is concerned with comparing various process technological routes in an integrated facility rather than end products, the basis for comparison will use the reference flow method [43], instead of functional units.

Inflow-outflow data for the Life Cycle Inventory was recorded from the Aspen Plus simulations, while the data for the specific GWP associated for each input and output was extracted from the Sima-Pro [46] database generated by the CML 2001 method [47]. Data for greenhouse gas emissions for the coal supply included the emissions from coal mining in South Africa, which was taken from Zhou *et al*. [48], and the emissions from the transport of coal were extracted from the GREET (The Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation) [49] database (Argonne National Laboratory, Chicago, USA). The ethanol production was assumed to replace an equivalent amount of gasoline [50], and the emissions resulting from that amount of gasoline (specific $CO_{2(eq)}$ taken from GREET [49]) was subtracted

Table 5 Data for inputs to MCE (US – United States; TDS – total dissolved solids; BFP – Basic Fuel Price; PPI – Producers Purchases Index)

Data for Static Value Inputs						
Item	**Cost Basis**	**Value**				
General Running Costs and Miscellaneous Expenses [52]	US$/litre	0.032				
Added Maintenance Costs of Recovery Boiler [28]	US$/litre	0.003				
Total Chemical Cost for 20% TDS	US$ (per annum)	2,850,292				
Total Chemical Cost for 30% TDS	US$ (per annum)	3,808,123				
Delivery Price of Coal to Sappi Saiccor (Personal Communication)	US$/ton	115.8				
Data for Stochastic Value Inputs						
	Electricity [57]	**Brazilian Ethanol [57]**	**US Ethanol [57]**	**BFP [58]**	**PPI [57]**	**Interest Rate [57]**
Year	**US$/kWhr**	**US$/l**	**US$/l**	**US$/l**		**%**
2003	0.032	0.252	0.337	0.245	124.8	15.16
2004	0.039	0.254	0.422	0.337	127.7	11.31
2005	0.044	0.375	0.463	0.535	132.4	10.64
2006	0.048	0.508	0.674	0.676	142.6	11.14
2007	0.04	0.467	0.524	0.604	158.2	13.08
2008	0.04	0.52	0.587	0.838	180.8	15.12
2009	0.045	0.45	0.449	0.474	180.7	11.8
2010	0.054	0.612	0.483	0.601	191.6	9.91
2011	0.087	0.867	0.683	0.836	207.6	9
2012	0.106	0.666	0.611	0.865	220.5	8.78

from the system emissions, as per the substitute method [43,50]. The method described in the Ecoinvent database manuals [51] was then used to calculate the overall emissions for the systems of each scenario. Regarding the interpretation, a positive NGHGR means that the integration of ethanol production reduces greenhouse gas emissions for the combined pulping-ethanol plant, while a negative value indicates that the integration of ethanol actually increases global warming.

Economic evaluation

The process models were used to construct financial models in order to assess the economic viability of the various technical scenarios considered. These financial models were based on Monte Carlo economics (MCE), so that the indicator of economic viability, such as the IRR or the MESP, is reported as an aggregated value that accounts for the effects of fluctuations on economic viability [52,53]. Thus, if the IRR is reported, which is primarily for comparing scenarios, it is an average value resulting from the numerous iterations involved in MCE. When the MESP is reported for the most technically and economically desirable scenario, it is reported as the selling price needed to produce an IRR of 25%, with a probability of 80% or more of achieving this IRR. An IRR of 25% represents the return level for private investment [54], while a failure rate of a probability of 20% is generally considered to be the maximum threshold for a target investor [55]. Detailed descriptions of the procedures that were followed for the capital estimation, establishment of the base financial model and implementation of MCE, and estimating economic parameters, are given in the support information file, as Additional file 1. The Simetar Excel Add-in [56] software (Simetar©, Texas, USA) was used for the Monte Carlo risk analysis.

The data used to populate the economic model is shown in Table 5 for the static and stochastic variables. Regarding fuel prices, it is not evident from the South African Biofuel Pricing Strategy (SABPS) [21] whether the pricing strategies developed for biofuels include second-generation ethanol from existing industrial process streams. Thus, an average first-generation ethanol price was calculated from United States- and Brazilian-based ethanol fuel prices, with no added premiums. In the section of the study where an MESP is calculated for the most desirable scenario, the future fluctuations of the basic fuel price (BFP) were simulated to base the forecasts of the future MESPs, because the SABPS stipulates that the first-generation biofuel price is related to the BFP. Thus, given that the future SABPS might include second-generation biofuels, the MESP calculated here is assumed to follow the projections of the BFP.

Additional file

Additional file 1: Economics Support Information File. This file is a Microsoft Word File detailing the methodology followed for establishing the economic model and super imposing a Financial Risk Assessment on the model.

Abbreviations

BFP: Basic Fuel Price; BTE: Biomass-to-Energy by Combustion; CaO: Calcium Oxide; CON: Conventional Distillation; GM: Genetically Modified; GWP: Global Warming Potential; IRR: Internal Rate of Return; ME: Multi-Effect Distillation; MESP: Minimum Ethanol Selling Price; MgO: Magnesium Oxide; NGHGR: Net Greenhouse Gas Reduction; SSL: Spent Sulfite Liquor; TCI: Total Capital Investment; TDS: Total Dissolved Solids; TPC: Total Polymeric Compounds.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

AMP is the primary author and investigator of the research in this paper. KH is the internal reviewer and brought the quality of English up to standard. JFG is the study group leader and approved the paper as a formal submission from the research group. All authors read and approved the final manuscript.

Acknowledgements

The authors would like to thank the National Research Foundation of South Africa for providing the funding for carrying out the study. We would also like to thank the process engineers at Sappi Saiccor, Colin Reddy and Brighton Chizwanza, for kindly providing technical information and arrangement of the sample shipment.

Received: 4 June 2014 Accepted: 13 November 2014
Published online: 05 December 2014

References

1. Ohgren K, Rudolf A, Galbe M, Zacchi G: **Fuel ethanol production from steam-pretreated corn stover using SSF at higher dry matter content.** *Biomass Bioenergy* 2006, **30**:863–869.
2. Martin N, Anglani N, Einstein D, Khrushch M, Worrell E, Price LK: *Opportunities to Improve Energy Efficiency and Reduce Greenhouse Gas Emissions in the U. S. Pulp and Paper Industry.* Berkeley, USA: Lawrence Berkeley National Laboratory; 2000.
3. Marinova M, Mateos-Espejel E, Jemaa N, Paris J: **Addressing the increased energy demand of a Kraft mill biorefinery: the hemicellulose extraction case.** *Chem Eng Res Des* 2009, **87**:1269–1275.
4. US Environmental Protection Agency: *Available and Emerging Technologies for Reducing Greenhouse Gas Emissions from the Pulp and Paper Manufacturing Industry.* North Carolina, USA; 2010.
5. Pimentel D: **Ethanol fuels: energy balance, economics, and environmental impacts are negative.** *Nat Resour Res* 2003, **12**:127–134.
6. Helle SS, Lin T, Duff SJB: **Optimization of spent sulfite liquor fermentation.** *Enzyme Microb Technol* 2008, **42**:259–264.
7. Nigam JN: **Ethanol production from hardwood spent sulfite liquor using an adapted strain of Pichia stipitis.** *J Biotechnol* 2001, **26**:145–150.
8. Marques AP, Evtuguin DV, Magina S, Amado L, Prates A: **Composition of spent liquors from acidic magnesium – based sulphite pulping of eucalyptus globulus.** *J Wood Chem Technol June* 2009, **2013**:37–41.
9. Helle SS, Murray A, Lam J, Cameron DR, Duff SJB: **Xylose fermentation by genetically modified Saccharomyces cerevisiae 259ST in spent sulfite liquor.** *Bioresour Technol* 2004, **92**:163–171.
10. Ogden J, Hochgreb S, Hylton M: **Steam economy and cogeneration in cane factories.** *Int Sugar J* 1990, **92**:131–140.
11. Bajwa PK, Shireen T, Aoust D, Pinel D, Martin VJJ, Trevors JT, Lee H: **Mutants of the pentose-fermenting yeast pichia stipitis with improved tolerance to inhibitors in hardwood spent sulfite liquor.** *Biotechnol Bioeng* 2009, **104**:892–900.
12. Quinteroa JA, Montoyaa MI, Sancheza OJ, Giraldoc OH, Cardona CA: **Fuel ethanol production from sugarcane and corn: comparative analysis for a Colombian case.** *Energy* 2008, **33**:385–399.

13. Crago CL, Khanna M, Barton J, Giuliani E, Amaral W: **Competitiveness of Brazilian sugarcane ethanol compared to.** *Energy Policy* 2010, **38**:7404–7415.
14. Robinson AL, Rhodes JS, Keith DW: **Assessment of potential carbon dioxide reductions due to biomass – coal cofiring in the United States.** *Environ Sci Technol* 2003, **37**:5081–5089.
15. Kumar A, Cameron JB, Flynn PC: **Biomass power cost and optimum plant size in western Canada.** *Biomass Bioenergy* 2003, **24**:445–464.
16. Miranda I, Gominho J, Pereira H: **Incorporation of bark and tops in eucalyptus globulus wood pulping.** *Bioresources* 2012, **7**:4350–4361.
17. Jantsch TG, Angelidaki I, Schmidt JE, Brana De Hvidsten B, Ahring BK: **Anaerobic biodegradation of spent sulphite liquor in a UASB reactor.** *Bioresour Technol* 2002, **84**:15–20.
18. Dias MOS, Ensinas AV, Nebra SA, Filho R, Rossell CEV, Regina M, Maciel W: **Production of bioethanol and other bio-based materials from sugarcane bagasse: Integration to conventional bioethanol production process.** *Chem Eng Res Des* 2009, **7**:1206–1216.
19. Cheng J, Zhou J, Liu J, Zhou Z, Huang Z, Cao X, Zhao X, Cen K: **Sulfur removal at high temperature during coal combustion in furnaces: a review.** *Prog Energy Combust Sci* 2003, **29**:381–405.
20. H-jiang H, Ramaswamy S, Al-dajani WW, Tschirner U: **Process modeling and analysis of pulp mill-based integrated biorefinery with hemicellulose pre-extraction for ethanol production: a comparative study.** *Bioresour Technol* 2010, **101**:624–631.
21. Department of Energy: *Preliminary Biofuels Pricing and Manufacturing Economics*. Pretoria, South Africa, 1–4
22. Sappi Group: *Saiccor Presentation*. KwaZulu-Natal, South Africa; 2011
23. Lobbes M, Fitznar HP, Kattner G: **High-performance liquid chromatography of lignin-derived phenols in environmental samples.** *Anal Chem* 1999, **71**:3008–3012.
24. Diedericks D, Rensburg EV, Görgens JF: **Fractionation of sugarcane bagasse using a combined process of dilute acid and ionic liquid treatments.** *Appl Biochem Biotechnol* 2012, **167**:1921–1937.
25. Canilha L, Carvalho W: **Ethanol production from sugarcane bagasse hydrolysate using pichia stipitis.** *Appl Biochem Biotechnol* 2010, **161**:84–92.
26. Alriksson B, Horvath I, Sjode A, Nilverbrant N, Jonsson L: **Ammonium hydroxide detoxification of spruce acid hydrolysates.** *Appl Biochem Biotechnol* 2005, **121–124**:911–922.
27. **ANDRITZ Sulfite Liquid Boiler (SulfitePower).** [http://www.andritz.com/products-and-services/pf-detail.htm?productid=13628]
28. Humbird D, Davis R, Tao L, Kinchin C, Hsu D, Aden A, Schoen P, Lukas J, Olthof B, Worley M, Sexton DD D: *Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol*. Colorado, USA: National Renewable Energy Laboratory; 2011.
29. Aden A, Ruth M, Ibsen K, Jechura J, Neeves K, Sheehan J, Wallace B, Montague L, Slayton A, Lukas J: *Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis for Corn Stover*. Colorado, USA: National Renewable Energy Laboratory; 2002.
30. Smith BB: *Economic Analysis of Hybrid Chiller Plants*. Atlanta, USA: American Society of Heating, Refrigerating & Air-Conditioning Engineers, Inc; 2002.
31. Mcaloon A, Taylor F, Yee W, Regional E, Ibsen K, Wooley R, Biotechnology N: *Determining the Cost of Producing Ethanol from Corn Starch and Lignocellulosic Feedstocks*. Colorado, USA: National Renewable Energy Laboratory; 2000.
32. Dias MOS, Modesto M, Ensinas AV, Nebra SA, Maciel R, Rossell CEV: **Improving bioethanol production from sugarcane: evaluation of distillation, thermal integration and cogeneration systems.** *Energy* 2011, **36**:3691–3703.
33. Dias MOS, Junqueira TL, Cavalett O, Cunha MP, Jesus CDF, Rossell CEV, Maciel R, Bonomi A: **Integrated versus stand-alone second generation ethanol production from sugarcane bagasse and trash.** *Bioresour Technol* 2012, **103**:152–161.
34. Department of Environmental Affairs and Tourism: *AQA Implementation: Listed Activities and Minimum Emission Standards. Draft schedule for section 21 Air Quality Act, Rev*. Pretoria, South Africa: Department of Environmental Affairs and Tourism; 2008.
35. Perin-Levasseur Z, Palese V, Marechal F: **Energy integration study of a multi-effect evaporator.** In *11th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Prevention (PRES)*. Prague, Czech Republic: PRES; 2008:1–17.
36. Aspen Technology Inc: *Aspen Plus®, Aspen Icarus®*, 2008. Massachusetts, USA, [http://www.aspentech.com/products/aspen-plus.aspx]
37. IChemE: *Pinch Point Analysis Spreadsheet*. Rugby, United Kingdom: Institution of Chemical Engineers; 2006 [http://booksite.elsevier.com/0750682604/?ISBN=0750682604]
38. Aspen: *Getting Started with Modelling Solids in Aspen Plus*; 2008. Massachusetts, USA, [http://www.aspentech.com/products/aspen-plus.aspx]
39. Nsaful F, Görgens JF, Knoetze JH: **Comparison of combustion and pyrolysis for energy generation in a sugarcane mill.** *Energy Conv Manage* 2013, **74**:524–534.
40. Nel S: *Catalytic Steam Gasification of Large Coal Particles*. Potchefstroom, South Africa: Northwest University; 1997.
41. Kuprianov VI, Arromdee P, Chakritthakul S, Kaewklum R, Sirisomboon K: **Combustion of some Thai agricultural and wood residues in a pilot swirling fluidized-bed combustor.** In *World Renewab Energy Confer*; 2011:148–155
42. Moor B: **Modern Sugar Equipment Assisting Cogeneration.** In *Proceedings of the South African Sugar Technologists' Association (SASTA) Congress*. Mount Edgecombe, South Africa: SASTA; 2008:1–13.
43. Melamu R, Von Blottnitz H: **2nd Generation biofuels a sure bet? A life cycle assessment of how things could go wrong.** *J Clean Prod* 2011, **19**:138–144.
44. Jimnez-Gonzlez C, Kim S, Overcash MR: **Methodology for developing gate-to-gate life cycle inventory information.** *Int J LCA* 2000, **5**:153–159.
45. Burgess AA, Brennan DJ: **Application of life cycle assessment to chemical processes.** *Chem Eng Sci* 2001, **56**:2589–2604.
46. PRé-Consultants: **SimaPro**. 2010. Amersfoort, The Netherlands, [www.pre.nl]
47. Rebitzer G, Ekvall T, Frischknecht R, Hunkeler D, Norris G, Rydberg T: **Life cycle assessment part 1: framework, goal and scope definition, inventory analysis, and applications.** *Environ Int* 2004, **30**:701–720.
48. Zhou PP, Lloyd P, Mzezewa C, Kipondya F, Asamoah J, Simonsen H: **Determination of regional emission factors for the power sector in Southern Africa.** *J Energy South Afr* 2009, **20**:11–18.
49. Wang M, Burnham A, Wu Y: *GREET*. Chicago, USA: Argonne National Laboratory; 2007 [https://greet.es.anl.gov/greet/index.htm].
50. Sheehan J, Aden A, Paustian K, Killian K, Brenner J, Walsh M, Nelson R: **Energy and environmental aspects of using corn stover for fuel ethanol.** *J Ind Ecol* 2004, **7**:117–146.
51. Hedemann J, König U, Cuche A, Egli N: *Technical Documentation of the Ecoinvent Database. Ecoinvent report no.4*. Dubendorf, Switzerland: Swiss Centre for Life Cycle Inventories; 2003.
52. Richardson JW, Lemmer WJ, Outlaw JL: **Bio-ethanol production from wheat in the winter rainfall region of South Africa: a quantitative risk analysis.** *Int Food Agribus Manage Rev* 2007, **10**:181–204.
53. Amigun B, Petrie D, Görgens J: **Economic risk assessment of advanced process technologies for bioethanol production in South Africa: Monte Carlo analysis.** *Renewab Energy* 2011, **36**:3178–3186.
54. Justice S: *Private Financing of Renewable Energy – A Guide for Policy Makers*. Nairobi, Kenya: United Nations Environment Programme (UNEP); 2009.
55. Hacura A, Jadamus-Hacura M, Kocot A: **Risk analysis in investment appraisal based on the Monte Carlo simulation technique.** *Eur Phys J* 2001, **B20**:551–553.
56. Richardson JW, Schumann K, Feldman P: *Simeter - Simulation & Econometrics to Analyze Risk*. Texas USA: Simetar, Inc.; 2008.
57. Petersen AM, Aneke M, Gorgens JF: **Techno-economic comparison of ethanol and electricity co-production schemes from sugarcane residues at existing sugar mills in Southern Africa.** *Biotechnol Biofuels* 2014, **7**:1–19.
58. **Department of Energy (South Africa) Website.** [www.energy.gov.za]

doi:10.1186/s13068-014-0169-8
Cite this article as: Petersen *et al.*: Techno-economics of integrating bioethanol production from spent sulfite liquor for reduction of greenhouse gas emissions from sulfite pulping mills. *Biotechnology for Biofuels* 2014 **7**:169.

Chapter 6: Integration of Gasification-Synthesis Processes in the Raw Sugar Industry

This chapter has been published in the journal "Bioresource Technology", volume 183, (2015) pages, 141–152 and can be found at http://dx.doi.org/10.1016/j.biortech.2015.02.007. It has been reproduced in this dissertation as is with the permission granted by the Elsevier Ltd publication house.

Title of Article: "Techno-economic assessment of integrating methanol or Fischer–Tropsch synthesis in a South African sugar mill"

Contribution of this Chapter

In this paper, the feasibility of integrating gasification-synthesis concepts into sugar mills using the sugarcane residues for methanol or Fischer-Tropsch syncrude production was explored. The design basis established in Chapter 4, which described the scale, residue costs and energy demands of the sugar mill applied to this chapter as well.

As the production of clean, compressed syngas for synthesis bears the primary costs of synthetic fuel production, the first objective was to optimise and compare the various technologies for syngas generation. Thereafter, synthesis flow sheets for methanol, FT syncrude production was constructed based on the syngas generation technology that operated on the most economical and technical optimum.

In relation to the overall objectives of this dissertation, it was shown that integrated methanol or FT synthesis was not currently feasible for sugar mills at their current efficiency and would therefore, not be an option for biofuel integration in the context of this dissertation since it

did not meet the criteria of self-sustaining processing or attraction for private investment. In terms of the objectives relating to flow sheet analysis, it was shown that coupling flow sheet analysis with statistical methods was an essential step in arriving at a an optimum set of operating parameters for the most costly sub-system of a process, and had allowed a fair basis for comparing alternative process technologies for a sub-system.

Authors' contributions

Abdul Petersen is the primary author and investigator of the research in this paper. Somayeh Farzad gave technical guide during the write-up, was the internal reviewer and assisted in structuring the paper. JFG is the study group leader and approved the paper as a formal submission from the research group. All the authors read manuscript and approved the integrity and accuracy of the results presented.

Bioresource Technology 183 (2015) 141–152

Contents lists available at ScienceDirect

Bioresource Technology

journal homepage: www.elsevier.com/locate/biortech

Techno-economic assessment of integrating methanol or Fischer–Tropsch synthesis in a South African sugar mill

Abdul M. Petersen, Somayeh Farzad, Johann F. Görgens *

Department of Process Engineering, University of Stellenbosch, Stellenbosch, South Africa

HIGHLIGHTS

- Integration of synthetic fuel production into sugar mills.
- Optimising syngas generation from biomass for cost and efficiency.
- Allothermal syngas production advantageous over autothermal.
- Conventional and advanced synthesis of Fischer Tropsch and methanol.
- Advanced methanol synthesis is the most favourable.

ARTICLE INFO

Article history:
Received 11 November 2014
Received in revised form 2 February 2015
Accepted 3 February 2015
Available online 17 February 2015

Keywords:
Optimising syngas production
Integrated biofuel synthesis
Techno economic assessment

ABSTRACT

This study considered an average-sized sugar mill in South Africa that crushes 300 wet tonnes per hour of cane, as a host for integrating methanol and Fischer–Tropsch synthesis, through gasification of a combined flow of sugarcane trash and bagasse. Initially, it was shown that the conversion of biomass to syngas is preferably done by catalytic allothermal gasification instead of catalytic autothermal gasification. Thereafter, conventional and advanced synthesis routes for both Methanol and Fischer–Tropsch products were simulated with Aspen Plus® software and compared by technical and economic feasibility. Advanced FT synthesis satisfied the overall energy demands, but was not economically viable for a private investment. Advanced methanol synthesis is also not viable for private investment since the internal rate of return was 21.1%, because it could not provide the steam that the sugar mill required. The conventional synthesis routes had less viability than the corresponding advanced synthesis routes.

1. Introduction

Lignocellulosic plant biomass can replace non-renewable carbon resources in numerous applications and has the potential to reduce greenhouse gas (GHG) emissions associated with present use of fossil fuels (Kreutz et al., 2008; Tijmensen et al., 2002). However, the conversion of lignocellulose into second generation biofuels comes at a significant cost of production, which has hindered its economic viability and prevented wide-scale commercial implementation (Sims et al., 2010). Bio-residues such as sugarcane bagasse and post-harvesting residues ("trash") in particular, are lignocellulosic materials generated in large quantities by the raw sugar industries (RSI) (Petersen et al., 2014; Leibbrandt et al., 2013). Thus, integrating biofuel production into this industry by converting lignocelluloses into biofuels and process energy could be economically attractive due to reduced costs of utilising residues onsite (Petersen et al., 2014), since the only costs associated with the bagasse is the amortised capital requirements for improving the mill efficiency while the costs of trash is associated with the collection from the field (Macrelli et al., 2012). As the export of energy products from a sugar requires an operating efficiency that is reflective of a steam demand of 0.4 tonnes per tonne of cane, the cost calculated for availing bagasse for such purposes was at 6 US$ per dry tonne (Petersen et al., 2014), which basically reflects the capital required to upgrade a typical South African mill that operates at a specific steam demand of 0.55 tonne/tonne cane. Thus, the installation of an integrated fuel co-production and energy cogeneration system would only be viable if it can meet the demands of the upgraded mill in a feasible manner (Macrelli et al., 2012).

Abbreviations: RSI, raw sugar industry; ALO-G, allothermal gasification; DFB, dual fluidised bed gasifier; ACE, amortised capital expenditure; CSP, cost of syngas production; HRSG, heat recovery steam generator; AUT-G, autothermal gasification; OOC, operational opportunity cost; SIF, supplementary information file; CE, conversion efficiency; FT, Fischer–Tropsch; IRR, internal rate of return.

* Corresponding author. Tel.: +27 21 808 3503; fax: +27 21 808 2059.
E-mail address: jgorgens@sun.ac.za (J.F. Görgens).

http://dx.doi.org/10.1016/j.biortech.2015.02.007
0960-8524/

The integration of biofuel production in the RSI has primarily been investigated for biological routes, where either the entire fraction of the lignocellulosic carbohydrates (cellulose and hemicellulose) is converted to biofuel, or just the hemicellulose fraction (Petersen et al., 2014; Macrelli et al., 2012). Where the cellulose and hemicellulose are converted, possible drawbacks include the high costs of the enzymes required to hydrolyse cellulose (Macrelli et al., 2012), where as using hemicellulose only results in a lower fuel yield (Petersen et al., 2014). Thermochemical conversion of lignocellulose to biofuels through gasification-synthesis is an alternative to biological conversion (Consonni et al., 2009). Gasification-synthesis would utilise both carbohydrates and lignin in the biomass feedstock for biofuel production and has shown to be more energy efficient (Leibbrandt, 2010). Intermediate liquid fuel products such as bio-methanol and bio-syncrude can take advantage of existing fuel production infrastructures, by processing with fossil based fuels at existing refineries, to produce Fischer–Tropsch (FT) liquids or biodiesel (Consonni et al., 2009). Previous investigations on the feasibility of finished FT liquids (i.e. gasoline and diesel) from biomass have shown that scales in excess of 110 dry tonnes per hour of feed are required for economic feasibility, due to the high capital investments (Leibbrandt, 2010). Such scales would not be attainable in the RSI of South Africa, since the average scale is at 300tons per hour of wet sugar cane, which results in a combined amount of trash and bagasse at 60 dry tonnes per hour (Petersen et al., 2014). Thus, the production of intermediate fuels may be an option for integrated biofuels scenarios using thermochemical pathways, since they are less capital intensive than facilities generating finished products (Ekbom et al., 2009).

The viability of integrating gasification-synthesis into an existing sugar mill is largely dependent (i) on the requirement for the gasification-synthesis process to meet the steam and electrical demands of the sugar mill, since this processing plant will replace the existing steam–electricity supply in the mill (Petersen et al., 2014), and (ii) the efficient conversion of lignocellulose into synthesis gas by gasification and conditioning, since this is where the primary capital and energy costs in a thermochemical process lie (Leibbrandt et al., 2013). As such, previous studies have analysed the effects of the gasification operating parameters (moisture content, pressure, temperature, steam-to-biomass ratio (SBR) and equivalence ratio (ER)) on the syngas composition and the gasification efficiency (Leibbrandt et al., 2013; Baratieri et al., 2008; Silva and Rouboa, 2014; Schuster et al., 2001) at thermodynamic equilibrium. The gasification efficiency measures the performance by relating the amount of input energy captured in the syngas while the syngas composition is important because the ratio of carbon monoxide and hydrogen determines the efficiency of methanol and FT syncrude synthesis (Leibbrandt et al., 2013; Phillips et al., 2011). Predictions made with thermodynamic equilibrium calculations (Schuster et al., 2001; Baratieri et al., 2008; Silva and Rouboa, 2014; Leibbrandt et al., 2013) have shown acceptable accuracy for biomass gasification at temperatures of 800–1000 °C, in the presence of a gasification or steam reforming catalyst (such as dolomite or nickel-based), which also reduces tar formation to an acceptable level (Filippis et al., 2004; Rapagna et al., 1998).

Coupling the measurement of gasification efficiency with equilibrium models, has been used in statistical models to optimize the operating parameters of syngas production for applications such as Fischer Tropsch synthesis and H_2 production (Leibbrandt et al., 2013; Silva and Rouboa, 2014). These studies however, have not considered the impact of downstream syngas conditioning units on the overall efficiency and furthermore, have not quantified the associated costs of producing syngas. As examples, the capacity of the heat recovery steam generator on the syngas stream and the energy demands of the Rectisol unit to remove the acids from syngas are directly dependent on the enthalpy and properties of the product gas (Kreutz et al., 2008; Leibbrandt, 2010), and thus – the efficiency and cost of conditioning syngas is dependent on the operating conditions of gasification. Otherwise, in terms of cost and efficiency, more efficient process technologies are often characterised by greater capital and operational expenses (Ryan and Campbell, 2012) in a general sense. With particular reference to syngas production, the combined gasification-conditioning processes can be configured for steam-blown or oxygen-blown gasification, with the latter having higher efficiency (Puig-arnavat et al., 2010), while being considerably more costly (Baratieri et al., 2008).

Thus, the present study assessed the techno-economic feasibility of methanol and FT bio-syncrude synthesis as alternative options for integrating biofuel processes into the RSI of South Africa. Operational conditions for gasification-conditioning to produce cleaned-compressed syngas were first simulated in Aspen Plus®, to minimise the overall production costs while maintaining an acceptable conversion of biomass to synthesis gas. The preferred gasification-conditioning approach was subsequently combined with methanol or FT synthesis flow-sheets through Aspen Plus® simulation (version 7.1) (Aspen Technology Inc., 2008). All Aspen simulations were based on published technical data and technologies. For both FT and methanol production, conventional and advanced synthesis technologies were compared on the basis of energy efficiency and economics. Generally, conventional synthesis technologies employs gas-phase reactors with recycle loops, while advanced synthesis technologies employs liquid-phase reactors that potentially operates on a once through basis. Financial risk assessments of the alternative flowsheets were completed with Monte Carlo (stochastic) methods, using Simetar™ (Richardson et al., 2008) software.

2. Methods

2.1. Technological overview

2.1.1. Lignocellulosic biomass gasification

Equipment designs for the gasification of lignocellulosic biomass tend to focus on fluidised bed gasifiers (Tijmensen et al., 2002), which can be based on autothermal gasification (AUT-G) or allothermal gasification (ALO-G). During AUT-G, the gasification medium includes both steam and an oxidant in sub-stoichiometric proportions, to initiate the combustion reactions and to supply the reaction heat required by the endothermic gasification (reduction) reactions (Filippis et al., 2004). A high calorific value of the syngas, as is desired for Fischer–Tropsch synthesis, requires the oxidation medium as pure oxygen. The pure oxygen is obtained by an Air Separation Unit, which typically bears substantial energy and capital costs (Kreutz et al., 2008; Schuster et al., 2001). AUT-G systems can also be done under pressure to avoid costly syngas compression for downstream synthesis applications (Larson et al., 2009). However, a pressurised system requires high capital cost and also reduces the content of hydrogen and carbon monoxide in the syngas (Holmgren et al., 2012).

Regarding ALO-G, a syngas with a calorific value similar to that of the oxygen-fed autothermal systems (Schuster et al., 2001) is produced by reforming with steam. The energy required for the endothermic steam gasification reactions is supplied by a heat transfer medium (bed material) that is circulated between combustion and gasification chambers in the setup of a dual fluidised bed gasifier (DFBG) (Schuster et al., 2001; Baratieri et al., 2008). The bed material containing the gasification catalyst is separated from the gasification chamber effluent (i.e. syngas) with unconverted char and enters the combustion chamber with additional fuel to heat the bed material that is returned to the gasifier. Un-reacted char, however, only occurs if the gasification conditions

are below the requirements of the carbon boundary point (CBP) (Baratieri et al., 2008). For biomass species, the CBP typically takes place at a molar H_2O to carbon (content of the biomass) ratio of approximately 0.5 (Baratieri et al., 2008), which in terms of the SBR for cane residues, amounts to 0.215 at temperatures that are below 750 °C. As gasification for synthetic fuel production usually takes place at higher SBRs (Leibbrandt et al., 2013) and temperatures; the presence of char entering the combustor will be minimal, implying that heat required for the gasification reactions would be sourced directly from biomass that is diverted to the combustor (Pfeifer et al., 2004). However, this can have a substantial effect of the overall efficiency with which the biomass is converted to syngas, notwithstanding the additional capital required for the combustor (Schuster et al., 2001; Baratieri et al., 2008).

2.1.2. Methanol synthesis

Conventional synthesis reactors for methanol synthesis entail a fixed bed gas phase reactor, over a copper/zinc/aluminium catalyst (Phillips et al., 2011; Hamelinck and Faaij, 2001), which is prone to sintering under high temperature. Thus, the conversion per pass of syngas is limited to about 30%, to control the heat generated by the exothermic synthesis reaction. To assist with the removal of heat from the reactor, a high recycle ratio of about 5:1 (mol flow mixed feed/fresh feed) of the un-reacted gases is needed (Hamelinck and Faaij, 2001). This mode of synthesis, however, incurs significant costs due to the compression of the recycle streams (Hamelinck and Faaij, 2001).

Advanced methanol synthesis reactors employ an inert liquid medium in which the catalyst is suspended and through which the syngas bubbles (Hamelinck and Faaij, 2001). Synthesis gas then defuses through the liquid medium to the catalyst and product gasses diffuse back through the medium into the gas phase. At the same time, a rapid transfer of the reaction heat from the catalyst through the liquid to a cooling mechanism occurs, enabling conversions of about 70% in a single pass (Hamelinck and Faaij, 2001).

2.1.3. FT synthesis

With conventional FT synthesis configurations, the conversion of syngas in a fixed bed gas phase reactor is limited to about 40% per pass, to control the heat generated by the exothermic synthesis reactions (Tijmensen et al., 2002; Dry, 2002). In order to purge the reaction heat from the reactor to avoid catalyst sintering and also to improving the overall FT product yield, recycle ratios for the un-reacted gases of 3:1 (mol flow mixed feed/fresh feed) have been reported (Tijmensen et al., 2002). The cost for this mode of synthesis however, is accentuated by the compression and reforming of the light hydrocarbon gases (C_1–C_4) to CO and H_2 in an Auto-Thermal Reformer (ATR), due to the additional capital and operating costs of the ASU and HRSG (Kreutz et al., 2008) that is associated with the reforming of recycle gas.

Under advanced modes of FT synthesis, the high pressure reactor conditions ensure that the wax products exist as a liquid phase in which the catalyst is suspended, which is removed from the bottom of the reactor (Tijmensen et al., 2002; Dry, 2002). Thus, as the reaction heat is rapidly dispensed through the liquid medium to a cooling medium, a syngas conversion of up to 90% per pass is possible (Dry, 2002; Ekbom et al., 2009), which invariably will reduce the residual syngas available to satisfy the energy demands of the adjacent sugar mill.

Depending on the desired product distribution, the operating schemes normally applied for FT synthesis (for both advanced or conventional configurations) are high temperature (HTFT), which operates at 300–350 °C and low temperature (LTFT) in the range of 200–250 °C (Dry, 2002; Ekbom et al., 2009). Low temperature (LTFT) catalysts are iron or cobalt promoted, and tends to generate products with high molecular weights that would require cracking at a refinery. While HTFT produces molecular weights that are mostly in the gasoline range, it also produces significant amount of oxygenates that destabilizes the synthetic crude, making hydrogenation of the product a necessary step for stabilization (Consonni et al., 2009). Since there is no significant production of oxygenates (Ekbom et al., 2009) in the LTFT product distribution, it would be suitable for bio-syncrude production.

2.2. Biomass characteristics and flow rates

The ultimate and proximate analysis for the various sugarcane residues considered in this study are presented in Table 1. The weighted average of values for bagasse and trash is presented, assuming a blending ratio of 1:0.58 (Petersen et al., 2014). The basis that the authors have previously used for integrating biofuel production into sugar mills (Petersen et al., 2014) via fermentation routes is considered here, as follows:

(i) An average sized South African mill have a total cane input of 300 wet tonnes/h, which results in a combined flow of trash and bagasse of 66.4 dry tonnes/h.
(ii) It is assumed that an older sugar mill has specifically been upgraded for more efficient steam and electricity usage, at 0.40 tonnes of steam and 41.64 kWe per tonne of cane. These cost for the refurbishment of the mill is accounted for through the amortising the capital expenditure, and assigning it as the price paid for bagasse at 6.3 US$/dry tonne.

2.3. Approach for simulating thermochemical processes in Aspen Plus®

The biomass feedstock is characterised in Aspen Plus® as a non-conventional component, in terms of its proximate and ultimate analysis. The gasification reactor (and combustion reactor in the case of allothermal gasification) is thus simulated as a component yield reactor model (RYIELD), followed by an RGIBBS model that predicts the composition of the syngas through thermodynamic calculations, by minimising the Gibbs free energy (Puig-arnavat et al., 2010). The heat of decomposition from the RYIELD is connected to the RGIBBS, in order to maintain the energy balance (Puig-arnavat et al., 2010), which implies that gasification system is treated adiabatically since the calculated flame temperature of the RGIBSS is the gasification temperature without any additional heat added to the system.

The energy demands of the supporting and gas-cleaning units within syngas production, such as the ASU was taken from Kreutz et al. (2008) at 380 kWh/tonne per tonne of oxygen

Table 1
Composition of residues considered for syngas production.

Case	Sugar cane resides		
Fuel	Bagasse	Trash	Aggregated cane residues*
Proximate analysis			
Fixed carbon	22.00	14.90	19.38
Volatiles	70.00	77.40	72.73
Ash	8.00	7.70	7.89
Ultimate analysis			
Ash	8.00	7.70	7.89
Carbon	44.32	39.80	42.65
Hydrogen	5.68	5.50	5.61
Nitrogen	0.00	0.20	0.07
Sulphur	–	–	–
Oxygen	42.00	46.80	43.77
Moisture	50.00	15.00	37.10

(a) Taken from Wienese (2001). (b) Taken from Jorapur and Rajvanshi (1997).
* The aggregate composition is based on the ratio of bagasse to trash of 1:0.58, as previously determined by Petersen et al. (2014).

required, while the demands for a single stage Rectisol was taken from Sun and Smith (2013) at 7.57 kW thermal and 1.42 kW electrical energy per kilo-mole of acid gas in the syngas (per hour). The total heat availability for steam generation from the syngas cooling was determined by simulating a heat exchanger with a dew-point specification, while required energy for the syngas compression to 33 bar Sun and Smith (2013) was modelled by three compressors with inter-stage coolers, each with mechanical and polytropic efficiencies of 90% and 80% respectively (Kreutz et al., 2008).

The reactor for methanol synthesis was treated like an RGIBBS reactor (Phillips et al., 2011; Hamelinck and Faaij, 2001), with the temperature and pressure specified according to literature. The FT synthesis reactor was simulated as stoichiometric reactions between CO and H_2, with three long-chained alkanes representing the various fractions of FT syncrude, such as C_9H_{20} for gasoline, $C_{15}H_{32}$ for diesel and $C_{21}H_{44}$ for waxes (Leibbrandt et al., 2013). The conversions for these reactions are sourced from literature.

The separation of residual gases from the crude synthesis products (in liquid state) was simulated as flash tanks, using the Redlich–Kwong–BM equation of state for methanol (Phillips et al., 2011) and the NRLT equation of state for FT bio-syncrude (Chen and Mathias, 2002). The separation of water from the alkanes in the case of FT was simulated with the Liquid–Liquid separator in Aspen Plus® using the Unifac-Liquid–Liquid model. The simulation of the power generation with the gas-turbine using unconverted/un-recycled syngas and the subsequent Combined (steam) Cycle was done as reported previously (Petersen et al., 2014; Kreutz et al., 2008).

2.4. Establishment of system boundaries

As this study concerns the integration of a biofuel process into a host industry, the boundary of the system studied extends over the entire biofuel production processes that are depicted in Fig. 2. Thus, it begins at the reception of bagasse from the mill and trash from the field, and extends till the final fuel products and the process steam/electricity that is returned to the mill for servicing the energy needs. If the energy needs of the mill is not met by the steam/electricity that is returned to the mill, the cost of supplementing the deficit is included in the boundaries of the system. Concerning the sub-system that is initially optimised for syngas production (depicted as Fig. 1A–C; and shown in Fig. 2A and B as the "Gasification and Syngas Clean-up" block), the boundaries extend from the reception of biomass till the point where clean and compressed syngas is generated.

2.5. Optimisation procedure for syngas production

2.5.1. Simulation of syngas production from catalytic biomass gasification in Aspen Plus®

The syngas production from lignocellulosic materials is presented in Fig. 1A for the atmospheric system (AUT-G (A)) and Fig. 1B for the pressurised systems (AUT-G (P)). Biomass is firstly dried to moisture contents of 5–25% with flue gas (Tijmensen et al., 2002), before being fed to the gasifier. Steam and oxygen (from the ASU) is fed to the gasifier, which is operated with SBRs and ERs in the ranges of 0.5–2.5 and 0.2–0.4 respectively. The solid ashes are removed by cyclones after the gasifier (Phillips et al., 2011) and the syngas is cooled in a HRSG to generate steam, while the ashes formed by condensing alkalis during the cooling is removed by a bag-filter (Tijmensen et al., 2002). The ashes are disposed as additives to the fertilizer on the cane fields. The syngas is then dehydrated in a series of knockout drums that alternates with the compression sequence, before acid gas removal in a Rectisol unit. In the case of the pressurised system, oxygen is initially

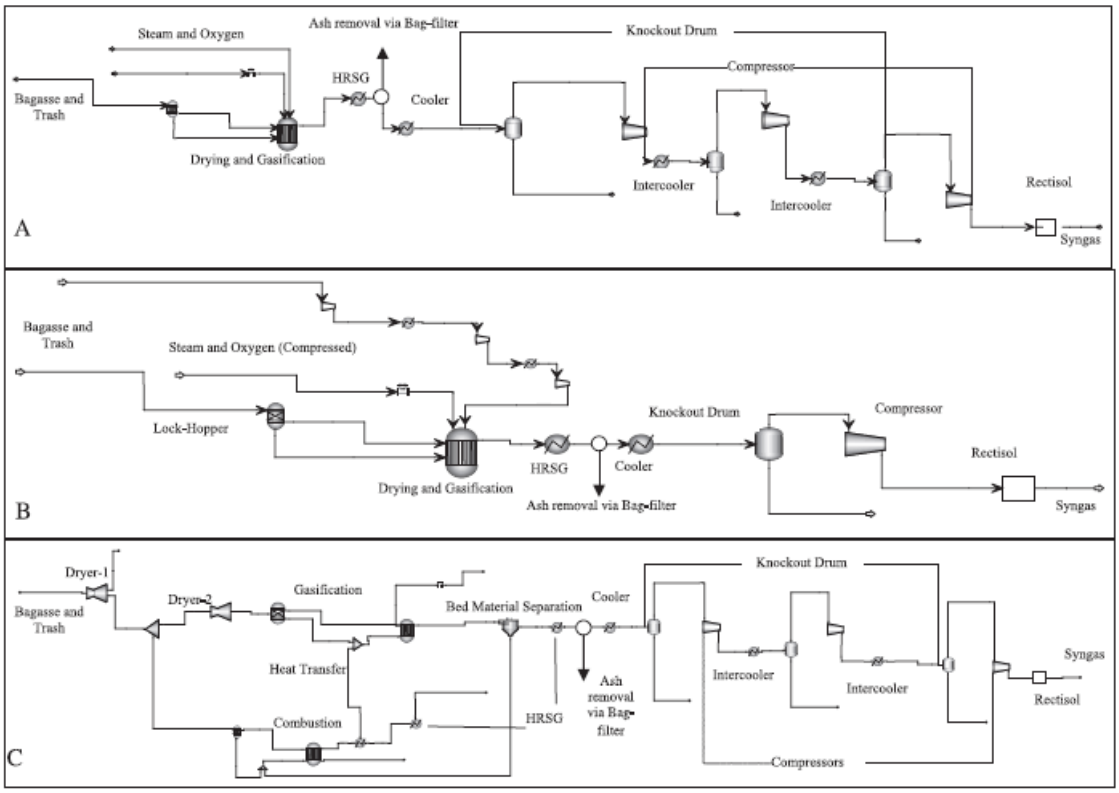


Fig. 1. Flow sheet of (A) autothermal atmospheric gasification; (B) pressurised autothermal gasification and (C) allothermal gasification.

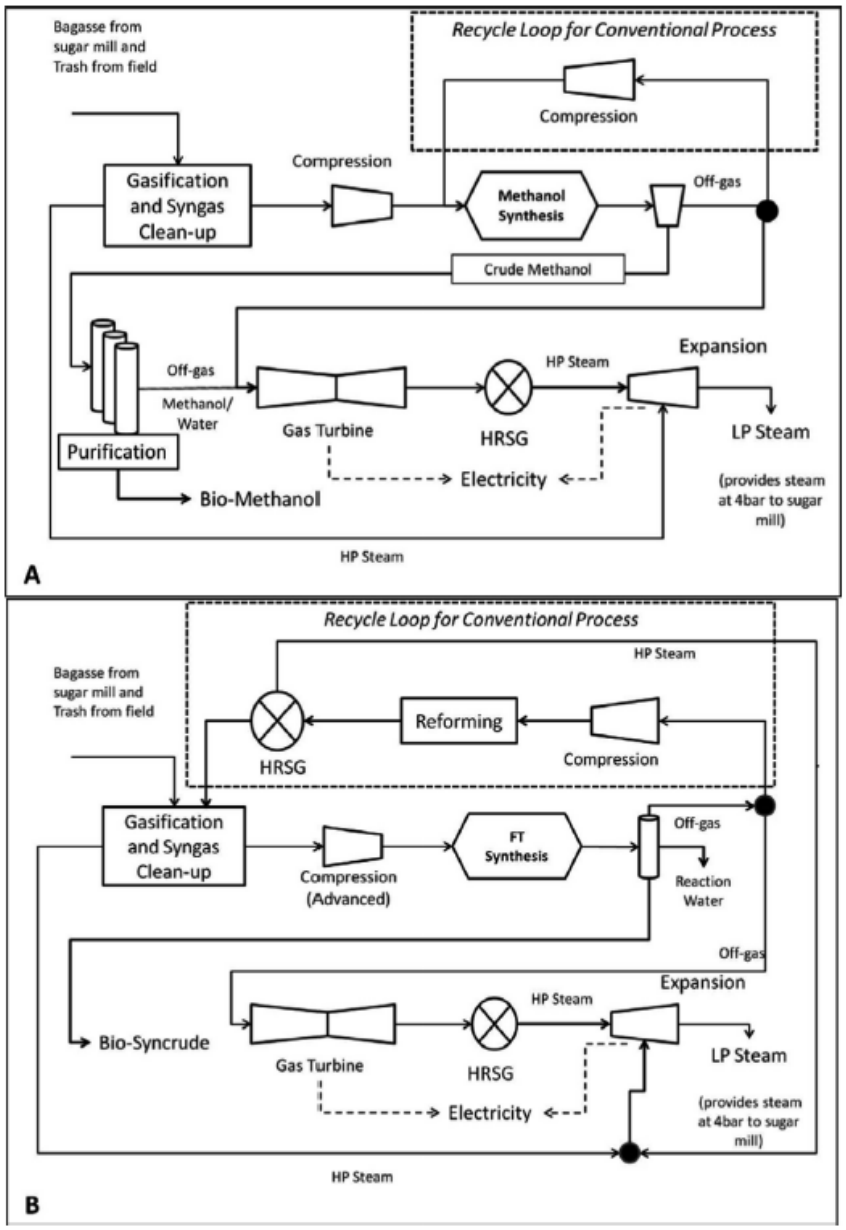


Fig. 2. Flow-sheets of synthetic fuel processes for: (A) methanol and (B) FT bio-syncrude. For both (A) and (B), the additional units required for the recycle loop in the conventional processes are shown in a dashed (–) line.

compressed to compensate for the gasification pressure 29.9 bar and the biomass is fed via a lock-hoper (Larson et al., 2009).

For allothermal gasification (Fig. 1C), biomass is initially dried in a primary drier to 25% moisture and then split between the gasifier and combustor, where a minimum moisture content of 25% is assumed to prevent self-ignition (average of the 30% recommended for bagasse fibres (Petersen et al., 2014), which is now mixed with trash fed at 15%). The biomass fraction for gasification is dried further to 5–25% moisture in a secondary drier, and then is blown into the gasifier with steam. The heated bed material containing a dolomite catalyst transfers heat from the combustor to the steam reforming reactions. The heat transferred by the bed determines the portion of biomass to be combusted, which was estimated from Schuster et al. (2001) at a range 0.4–0.6 in order for the temperature of the gasification chamber to be above 900 °C (Pfeifer et al., 2004) for tar free syngas. After gasification, the bed material is separated from the syngas via cyclones and the syngas undergoes cooling for steam generation, dewatering and compression to be processed in a Rectisol unit.

The modelling of the heat transfer was simplified, since the primary concern was to conserve the energy balance to ensure the correct temperature of the allothermal gasification. Thus, the heat transfer duty from the combustion reactions to the gasification via the circulating bed material was simulated as a heat stream. The combustor was simulated adiabatically with a heat exchanger on the exhaust gas and the heat stream connects this heat exchanger to the gasifier. The heat transfer is simulated by cooling down the flue gas from the adiabatic combustion temperature of the flue gas to a temperature that is 70 °C higher than the gasification chamber temperature (March, 1998), using the Design Specification feature

in Aspen Plus®. After heat transfer with the bed material, the flue gas is cooled to 250 °C in an HRSG and then is used for dehydrating biomass. In order to validate the simulations for the various modes of gasification, the predictions of syngas compositions were compared to experimental literature, using the reported operating conditions and biomass characteristics. The validation runs for AUT-G was performed with data given in Filippis et al. (2004), while ALO-G validation was performed with data from Rapagna et al. (1998) and Chen et al. (2010).

2.5.2. Description and calculation of optimisation variables

2.5.2.1. Cost of syngas production (CSP). The CSP relates the overall cost of production to the sum of the amortised capital expenditure (ACE) of the equipment over an economic period of 20 years (N) and opportunity cost of the operating expenditure to the chemical energy of the syngas (product of the syngas flow rate and lower heating value). The ACE is calculated from the total installation costs (TC) of all the syngas production equipment using the amortisation formula (The Institute of Electrical and Electronics Engineers Inc., 2002) that is shown by Eq. (1) average interest rate (r) of 11.6%.

$$\mathrm{ACE} = \frac{r * \mathrm{TC} * (1+r)^N}{(1+r)^N - 1} \quad (1)$$

where ACE – amortised capital expenditure; TC – total installation cost; r – average interest rate of 11.6%; N – period of economic analysis, 20 years.

The operating opportunity cost (OOC) represents the cost incurred that results from using electricity and steam for syngas production. Macrelli et al. (2012) for example identified an OOC for integrating second generation ethanol production into the cane-ethanol industry as a loss in the potential sale of export electricity resulting from the increased energy demands of second generation ethanol production when compared with only generating electricity. A similar approach is adopted in the present study, where use of electricity and steam for syngas production is considered as an operating opportunity cost incurred. It should be noted that the OOC could take a negative value, if the thermal heats released from the exothermic processes bears potential revenues that exceeds the energy demands.

To calculate the OOC, it is thus considered that the thermal heat of the high pressure (HP) steam used in syngas production could potentially have been used to generate electricity at an efficiency of 27%, while the low pressure (LP) steam could have been generated at an efficiency of 10%. These values for efficiency were calculated using an Aspen Simulation of a heat recovery steam generator (HRSG), where the heat resulting from the cooling of a hypothetical syngas at 800 °C was used to generate high pressure steam that was expanded through turbines from 124.1 bar to low pressure steam at 4 bar and then exhausted in a condensing turbine to 0.2 bar. Thus, the electrical equivalent of the net steam demand or generation is summed with the direct use of electricity, and the AMC to derive the expression for CSP as shown by Eq. (2). The unit price of electricity used in this calculation was 0.18US$/kWh, the average of the values forecasted over the period 2012–2029, using a linear trend of the historic prices presented for electricity in a previous study of the authors (Petersen et al., 2014).

$$\mathrm{CSP} = \frac{(0.29 * (\mathrm{HP_{SBR}} - \mathrm{HP_{Generated}}) + \mathrm{Electricity} + \mathrm{LP} * 0.1) * \mathrm{E_{Price}} + \mathrm{Feedstock_{Purchases}} + \mathrm{ACE}}{\mathrm{Syngas\ chemical\ energy}} \quad (2)$$

where CSP – cost of syngas production; $\mathrm{HP_{SBR}}$ – high pressure steam consumption of SBR; LP – low pressure steam; E_Price – electricity price

2.5.2.2. Temperature. The gasification temperature is the adiabatic flame temperature calculated from the predicted (equilibrium) syngas composition, and is thus dependent on optimization of operating conditions. The amount of tar present in the syngas depends on the gasification temperature under catalytic conditions. Thus, the temperature required for tar-free (or acceptable tar level) is 800 °C and 900 °C for the atmospheric (Filippis et al., 2004) and pressurised AUT-G respectively, and 900 °C for the allothermal gasification systems (Pfeifer et al., 2004).

2.5.2.3. H_2/CO ratio. In order to promote efficient conversion of syngas to methanol or synthetic FT crude, the ratio of H_2 to CO was always maintained as two (Leibbrandt et al., 2013; Phillips et al., 2011).

2.5.2.4. Conversion efficiency (CE). This efficiency describes the extent to which the calorific energy in the feed stock was captured as H_2 and CO in the syngas, as shown in Eq. (3).

$$\mathrm{CE} = \frac{\mathrm{HoC_{H_2}} * \mathrm{Flow_{H_2}} + \mathrm{HoC_{CO}} * \mathrm{Flow_{CO}}}{\mathrm{LHV_{Feed\ stock}} * \mathrm{Flow_{Feedstock}}} \quad (3)$$

where CE demonstrates conversion efficiency, $\mathrm{HoC_{H2}}$ and $\mathrm{HoC_{CO}}$ stand for specific heat of combustion of hydrogen; and carbon monoxide respectively and LHV shows lower heating value.

2.5.3. Gasification-conditioning optimisation for syngas production

Extending the approaches formulated by Leibbrandt et al. (2013) and Silva and Rouboa (2014), equilibrium-based modelling with various combinations of the gasification parameters in a 3^3 factorial design, as presented in Table 2, was used to simulate the effects of moisture, SBR and ER (biomass split for ALO-G) on the combined gasification-condition systems for syngas production. The factorial design was implemented in Aspen Plus® using the Sensitivity Model Analysis tool. The data recorded from the simulations that were carried out in the factorial design included the syngas compositions, process and utility stream flows and the energy demands of the units. The data was then processed to calculate the values of the optimisation variables defined (such as CE, syngas ratio and CSP), in order to perform a multi-variable regression analysis using the Simetar® Add-in for MS Excel. For each optimisation variable, regression analysis was performed using the form of Eq. (4) for the predicted response variable, Y_j (j = CSP, Temperature, H_2/CO, CE), in terms of the input variable, X_i (where i = Moisture, SBR and ER or mass split). Using the MS Excel Solver Add-in, the optimisation of the gasification parameters was performed by maximising the CE, while minimising the CSP with equal weights in a uni-variable objective function approach (Silva and Rouboa, 2014), subject to the constraints of the H_2/CO ratio and temperature.

$$Y_j = \sum L_i * X_i + \sum \mathrm{IP}_n * X_i X_{i-1,+1,+2} + \sum Q_i * X_i^2 \quad (4)$$

Table 2
Parameters for optimisation of syngas production options.

	Input parameters				Constraints	
	Moisture	SBR	ER	Split	H_2/CO	Temperature (°C)
AUT-G	0.05–0.25	0.5–2.5	0.2–0.4	–	2	800 (A), 900 (P)
ALO-G	0.05–0.25	1–3	-	0.35–0.6	2	900

2.6. Process flow descriptions for synthesis simulations

2.6.1. Methanol Synthesis and Purification

The methanol synthesis process flow diagram is shown in Fig. 2A. The conditioned synthesis gas from the Rectisol unit enters the methanol synthesis section, where it is either compressed to 60 bar (Phillips et al., 2011) for the conventional (gas phase) synthesis or 98 bar for the advanced (liquid phase) synthesis reactor (Hamelinck and Faaij, 2001). In the conventional system, a small portion of the feed is heated to the reaction temperature of 300 °C (Phillips et al., 2011) and enters the reactor to initiate the reactions, and then the bulk of the reacting feed enters. The temperature of the reactor product is then decreased to 45 °C, firstly by generating saturated steam at 4 bar and subsequently with cooling water, and then flashed at 38 bar to remove the un-reacted gasses (Phillips et al., 2011). 87% of the un-reacted gases are recompressed and recycled back to the synthesis reactor, to maintain the required recycling ratio for reactor temperature control (Phillips et al., 2011). The advanced reactor differs from the conventional synthesis in that the reactor feed is pre-heated to the reaction temperature of 250 °C, which is isothermally maintained by steam generation (Hamelinck and Faaij, 2001). Furthermore, cooling of the reactor effluent is achieved by heating up the reactor feed directly, and none of the un-reacted gases are recycled once the product is degassed.

For purification (Dijk et al., 1995) of the crude methanol product, the dissolved gases are firstly removed in a Toppings column that has 32 trays. The bottoms product is subsequently distilled in a column under 6.5 bar pressure of containing 30 trays, to produce about 50% of the purified methanol product. The bottom of this column is then flash-fed into an atmospheric column having 65 trays that produces the remaining portion of the methanol product, and a combustible mixture of water and methanol.

2.6.2. Fischer–Tropsch synthesis and bio-syncrude separation

The FT synthesis process flow diagram is shown in Fig. 2B. The conventional technology uses a gas phase-fixed bed reactor operating at 23.5 bar at 240 °C in the low temperature scheme to ensure that all the reaction products remain in the gas phase (Ekbom et al., 2009; Tijmensen et al., 2002). A conversion per pass of 40% of the CO to hydrocarbon compounds is assumed (Tijmensen et al., 2002). The reactor effluent is cooled by generating saturated steam at 4 bar, followed by cooling to 45 °C with cooling water, to separate the gaseous products, un-reacted gases and water from the FT liquid product mix, which forms the bio-syncrude. Of the gaseous stream, 70% is split and compressed to 33 bar for auto-thermal reforming with steam and oxygen (Kreutz et al., 2008). The amount of the steam added to the reformer is at a molar ratio of 1:1 (Ozkara-Aydınoglu, 2010), with the hydrocarbon gases and the oxygen fed to maintain the ATR reactor temperature at 1000 °C (Leibbrandt et al., 2013) and the syngas generated by the ATR is then cooled in a HRSG before returning to the Rectisol unit.

The advanced slurry FT reactor also operates in the low temperature regime at 40 bar and 240 °C, while its once-through conversion per pass is specified as 80% (Kreutz et al., 2008). Regarding the product distribution of the hydrocarbons formed, an equal distribution between the four product types (i.e. gases, naphtha, diesel and waxes) was specified, which occurs at the assumed probability of 90% on the Anderson–Schulz–Flory distribution (Ekbom et al., 2009).

2.6.3. Power utilities and heat integration

All the un-recycled off-gases generated by both the FT and methanol processes were used to generate steam and electricity via a gas turbine followed by an HRSG. The gas turbine had a pressure ratio of 19.5 bar and thus, all streams entered the gas turbine at 23.5 bar to account for pressure drops across the nozzles (Kreutz et al., 2008; Petersen et al., 2014). The amount of air used for the combustion was specified using a Design Spec, such that the exhaust gases of the turbine were at 650 °C. Steam was then generated 124 bar and expanded to 4 bar for the utility requirements of the gasification-synthesis processes and the adjacent sugar mill, while the excess steam was expanded till 0.2 bar (Kreutz et al., 2008; Petersen et al., 2014).

In order to integrate the exothermic heat of the gasification-synthesis processes into the adjacent sugar mill, a heat transfer medium (March, 1998) of low pressure steam at 4 bar was employed to transfer the heat. This pressure was selected since it represents the typical heating utility applied in the RSI in South Africa (Petersen et al., 2014). This heat integration strategy was considered in addition to the generic heat integration steps employed, such as heating the reactor feed streams with the product streams around the synthesis units (Leibbrandt et al., 2013; Kreutz et al., 2008). In order to avoid the capture of low quality heat, steam was generated by cooling hot streams such as compressor and reactor effluents to a temperature of 105 °C. This temperature was the dew-point temperature of the pressurized syngas, and was well below the dew points of the methanol and FT low molecular weights compounds in the reactor effluents. These dew points were estimated at 205 °C (40 bar, methanol) and 167 °C (20 bar, pentane), respectively, with the Clausius–Clapeyron Equation. Cooling below 105 °C is accomplished with cooling water at 30 °C, circulated through a cooling tower that operates with a Coefficient of Performance (COP) of 11.95. This is a conservative value of the COP, estimated using the method derived from literature (Morvay et al., 2009).

2.7. Financial risk assessment

Financial risks models were constructed, using the mass and energy balances, calculated utility requirements and equipment sizing from the Aspen Plus® simulations, to evaluate the economic viability of each gasification-synthesis process scenario. The capital costs of major process units were sourced from the estimates, while the minor/generic equipment costs were calculated by Aspen Icarus. Economic models included income statements, cash-flow statements and balance sheets for each process scenario, to calculate the internal rate of return (IRR).

A probabilistic simulation of the variables in these models was then imposed on the model (Richardson et al., 2007; Petersen et al., 2014), with the resulting IRR values as a stochastic distribution of possible outcomes, tested for probability of achieving the minimum threshold of 25%, as is required for private investment (Petersen et al., 2014). Process scenarios were deemed to be

economically unviable if the probability of achieving the threshold IRR was less than 80% (Petersen et al., 2014). This procedure for determination of economic viability has been described previously (Petersen et al., 2014), and follows the procedures detailed in the appendix of (Richardson et al., 2007).

3. Results and discussion

3.1. Optimisation of syngas production

Fig. 3 demonstrates a good agreement between the syngas composition, predicted by the simulations of the autothermal and allothermal gasification systems, and the measured syngas compositions reported under the same operational conditions. For example, the allothermal gasification the Design Spec feature in Aspen Plus® predicted that 49.7% of the biomass feed would be required for direct combustion, to supply sufficient heat and maintain the gasification temperature at 830 °C. This result was similar to the measured values of Schuster et al. (2001), where 42.6% of the carbon in the primary feed was burnt to provide the reaction heat to sustain a gasification temperature of 800 °C in a DFB.

Table 3 shows the optimal conditions for the AUT-G and ALO-G systems for syngas production, as predicted by Aspen Plus® simulations. The efficiency of the atmospheric AUT-G system was 1.32 and 1.18 times greater than the allothermal and pressurised counterparts, respectively, meaning that the AUT-G yielded a greater amount of chemical energy in the form H_2 and CO per unit of biomass feedstock. Pressurised gasification resulted in high methane contents in the syngas, since high pressures favour the reverse of the steam reforming reaction. Low efficiency in the ALO-G system occurred because 42.0% of the biomass was required for direct combustion in order to sustain the temperature of the gasifier above 900 °C, for a tar free syngas. Thus, AUT-G systems are more efficient as the heat generated by the oxidation reactions are transferred directly to the endothermic reforming reactions, whereas the configuration of the ALO-G systems incurs significant losses of combustion heat in the flue gas.

Despite higher efficiencies, the cost of conditioned syngas production via the AUT-G systems was on average 1.8 times more expensive than the ALO-G counterpart. Fig. 4 depicts the comparison of the breakdown of the specific CSPs of each gasification system, indicating that the primary costs incurred by the autothermal system was the electricity costs (73% of total cost) of the ASU, the compressor (in the atmospheric case) and the Rectisol unit. Electricity costs of the atmospheric AUT-G system were 2.5 times higher than pressurised gasification, due to increased requirement for down-stream compression of syngass. Production costs of the ALO-G system were reduced by cooling the syngas and combustor stack gas by high pressure steam generation from the HRSG, which equivalently generates electricity in excess of the syngas conditioning requirements, once the gasification steam demand was withdrawn.

The amortised capital costs of the ALO-G and pressurised AUT-G system were slightly higher than the atmospheric AUT-G system, due to capital costs incurred by the combustor and the additional steam generator of the ALO-G and the increase in the costs of pressurised gasification equipment. Thus, while the AUT-G system incurs capital costs by the installation of the ASU, the ALO-G system incurs capital costs from the equipment associated with generation of thermal energy. The contribution of feedstock purchases to the overall CSP is in accordance with the conversion efficiency of

Table 3
Results for optimisation of syngas production scenarios for sugarcane lignocellulose.

Biomass	Cane residues		
Mode of syngas generation	AUT-G (A)	AUT-G (P)	ALO-G
Optimised operating parameters			
Steam to biomass	0.76	0.94	1.00
Moisture content (%)	10.80	6.44	5.00
Equivalence ratio	0.20	0.20	–
Biomass split	–		42.0%
Optimised objective variables			
Specific costs (US$/GJ)	10.99	7.75	4.30
H_2/CO	2.18	2.09	2.19
Gasification temperature (°C)	775.01	881.07	906.81
Conversion efficiency (%)	86.00	77.23	65.02
Correlation coefficients			
Specific costs	0.99	0.94	0.99
H_2/CO	0.92	0.97	0.97
Gasification temperature	0.99	0.98	1.00
Conversion efficiency	0.93	0.85	1.00

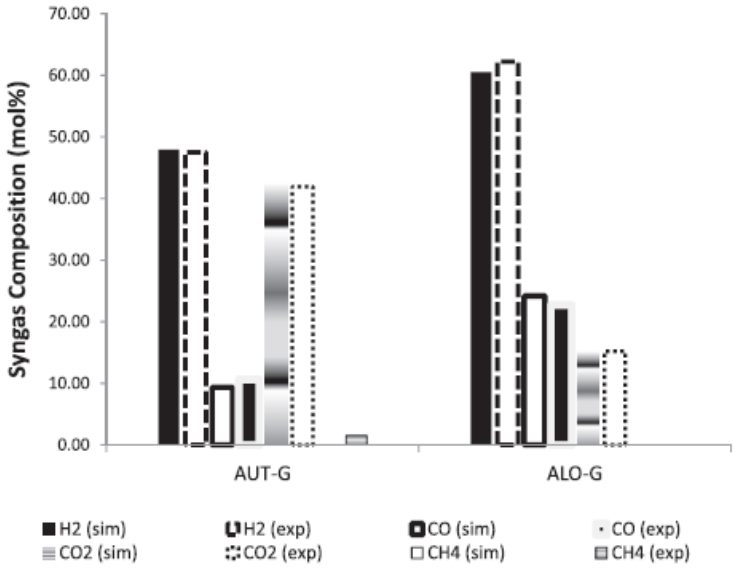


Fig. 3. Comparison of the syngas composition predicted by the models developed and respective experimental data (AUT-G (Filippis et al., 2004); ALO-G (Rapagna et al., 1998).

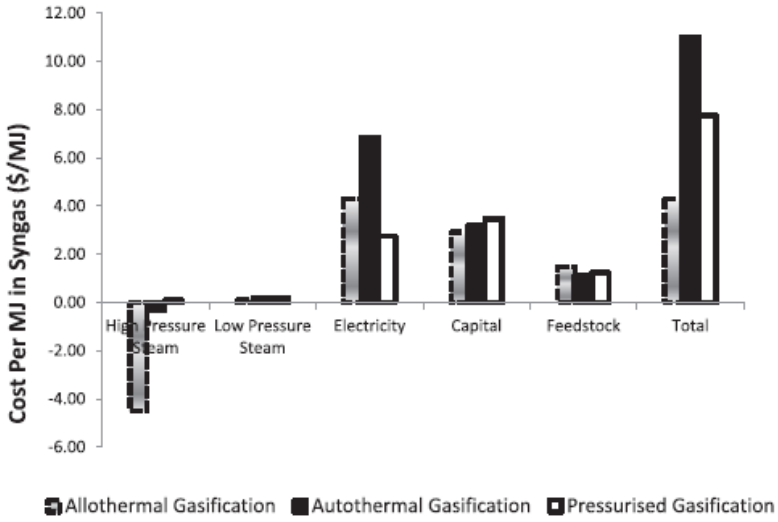


Fig. 4. Breakdown of CSP from the sugar cane residues.

the gasification routes. As atmospheric AUT-G had the highest conversion efficiency, the denominator in Eq. (2) had the highest magnitude, reducing the impact of feedstock purchases per GJ of syngas produced.

3.2. Techno-economic results

Table 4 compares the fuel production and steam/electricity generation of the gasification-synthesis processes to the combined utility demands of the integrated sugar mill and gasification-synthesis production process. The process described in Table 4 utilised the preferred allothermal gasification configuration. In some of the process scenarios, the steam supply from the gasification-synthesis process was insufficient to meet the combined utility demands of the integrated facility, in which case the deficits were met by either (i) purchasing electricity and producing steam by means of electric boilers, or (ii) purchasing natural gas to supplement the feed of the gas turbine or (iii) diverting syngas to the gas turbine. The overall technical performance was measured in terms of the net export efficiency (η_{ex}), as described by Eq. (5).

$$\eta_{ex} = \frac{\mathrm{HHV_{fuel}} + \mathrm{Electricity_{export}}}{\mathrm{HHV_{biomass\ and\ natural\ gas\ inport}} + \mathrm{Electrcity_{Import}}} \quad (5)$$

The yield of fuel energy from syngas for methanol production exceeded that of the FT synthesis by 37.1%, relatively (Table 4). This can be explained by referring to the fundamental reactions involving syngas for methanol ($CO + 2H_2 \rightarrow CH_3OH$) and FT liquids ($CO + 2H_2 \rightarrow -CH_2- + H_2O$), which shows that the water formation in FT synthesis results in a loss of chemical energy. Conversely, the amount of thermal heat generated by the methanol synthesis process was not adequate to meet the utility demands of the integrated sugar mill-gasification-synthesis facility, whereas the FT process generated steam in excess of utility demands, and was able to export electricity as sales (Table 4). The maximum amount of electricity exported was for the conventional FT scenario and it amounted to 47 kW per tonne of cane. Compared to the exports of 295 kW per tonne of cane where the residues are efficiently converted to heat and power, it is 6-fold less (Petersen et al., 2014).

The FT-advanced synthesis scenario yielded 45.1% more liquid fuel than the FT-conventional synthesis, while the latter exported 50.1% more electricity – due to both the increase in unconverted syngas available for heat and power generation, and the steam produced by reforming of the synthesis recycle gas stream. The advanced methanol synthesis scenarios yielded 14.0% more fuel than the conventional synthesis scenario, while also reducing the deficit of steam utility supply by 24.1%. The latter was due to the

Table 4
Technical results showing fuel and electricity outputs and imports and steam generation (E – electricity import; NG – natural gas import; D – diversion of syngas).

	Fischer Tropsch		Methanol (E)		Methanol (NG)		Methanol
Scenarios	Conventional	Advanced	Conventional	Advanced	Conventional	Advanced	Advanced (D)
Net outputs/inputs (<0 indicates import)							
Fuel production (l/h)	6500	9433	21,642	24,679	21,642	24,679	21,395
Fuel output ($MW_{thermal,HHV}$)	70	101	109	125	109	125	108
Electricity production (MW)	14.04	7.00	−4.06	−3.08	8.27	5.53	7.68
Total calorific output	83.61	107.95	105.17	121.47	117.50	130.09	115.66
Methane (tonnes/h)	0.00	0.00	0.00	0.00	−1.42	−1.01	0.00
Steam generation and requirements							
Total Steam Generation (tonnes/h)	165.53	150.86	110.86	113.71	121.95	121.87	121.07
Mill steam demand (tonnes/h)	120.00	120.00	120.00	120.00	120.00	120.00	120.00
Steam excess/deficit (–)	45.53	30.86	−9.14	−6.29	1.95	1.87	1.07
Electricity generation and requirements							
Gross electricity generation (MW)	81.53	64.48	67.26	55.93	84.23	68.15	71.59
Fuel electrical utilities (MW)	−55.00	−44.99	−53.04	−42.53	−63.47	−50.13	−51.43
Electricity needed for providing steam deficit	0.00	0.00	−5.80	−3.99	0.00	0.00	0.00
Mill electricity demand (MW) export	−12.49	−12.49	−12.49	−12.49	−12.49	−12.49	−12.49
Net energy efficiency	25.31%	32.68%	32.66%	37.36%	33.48%	37.71%	35.01%

cooling duty of the advanced synthesis reactor, due a higher conversion of the exothermic reaction, resulting in more LP steam generation. Furthermore, the advanced methanol synthesis also abated the electricity requirement for compression of the unconverted syngas in the synthesis recycle loop. The combined effects caused by the increase in yield/extent in the advanced synthesis process thus increased the yield of chemical energy in the fuel product and also improved the availability of utilities.

Focusing on the variances in the advanced methanol scenarios, making up the deficit in steam supply was the most feasible by importing natural gas for the overall efficiency. While importing excess electricity is the least efficient, diverting the syngas reduces the liquid yield by 15%. Supplying the amount of natural gas required for the overall steam demand increased the production capacity of both the gas turbine and the combined cycle for electricity production, resulting in an export of surplus electricity. As natural gas was needed at 4% of the total calorific input, the potential for greenhouse gas reduction of the output is reduced by 4%. This means that of the total calorific output 130.09 MW, an amount of 124.89 MW serves to replace fossil based energy and this amount is still in excess of the other scenarios.

The liquid fuel yields obtained from the simulations in the present study are compared to yields reported for similar process models (Fig. 5). The FT liquid yields of the advanced scenario determined by .(Larson et al., 2009) were greater by a factor of 1.2 than that of the simulation. This is due to the autothermal pressurised gasification that was used by Larson et al., 2009, which would increase the yield of syngas from biomass by a factor of 1.18, by referring to the differences in the conversion efficiency in Table 3 between AUT-G (P) and ALO-G. For the conventional FT synthesis, Tijmensen et al., 2002 used autothermal gasification and a high recycle ratio which show improved the yield by increments of about 9% and 5% compared to this study Furthermore, Tijmensen et al., 2002 had a selectivity of the syngas conversion in the FT reactor towards liquid products at 91%, which contributed a further 15% to the overall improvement of the liquid fuel yield, since this study only used a selectivity of 75%. Operating with high recycle as per Tijmensen et al. (2002) would not be suitable for integration of gasification-synthesis with a sugar mill, as it will result in a deficit of approximately 30% in the supply of steam utility to the sugar mill. Furthermore, the capital costs of the equipment involved in syngas recycling (ATR, ASU and HRSG) will be accentuated.

The liquid yields for the advanced methanol synthesis scenarios obtained in the present simulation were near identical to the values reported previously (Fig. 5), except for a few process-specific differences. The application of autothermal pressurised gasification (instead of allothermal gasification) by Hamelinck and Faaij (2001) should have increased the liquid fuel yield, but this was not achieved due to insufficient CO_2 removal in the syngas washing unit, resulting in a sub-optimal stoichiometric content of hydrogen in the synthesis gas that decreased the methanol yield. The liquid fuel yield for conventional methanol synthesis in the present simulations was 1.55-fold lower than reported by Hamelinck and Faaij (2001). Hamelinck and Faaij (2001) utilised pressurised, autothermal gasification, which has a 1.2-fold greater conversion efficiency than the allothermal used in the present simulation. Furthermore, Hamelinck and Faaij (2001) operated the conventional reactor at 250 °C as opposed to 300 °C used in this study, which had favoured a higher methanol conversion.

The economic viabilities of alternative process scenarios evaluations were affected by process intensification in synthesis steps (conventional vs. advanced) and the requirement for importing external energy sources to meet utility demands, such as the case with methanol synthesis scenarios (Fig. 6). The highest capital investment of 363.5million US$ was associated with the FT-conventional scenario, mostly due to the extra costs associated with the synthesis recycling loop, which is the ATR and the ASU for providing the oxygen. The conversion efficiency of this process was the lowest of all the scenarios considered, and also corresponded to the lowest IRR, at 9.7%. The TIC of the conventional-FT scenario was 20.0% higher than the advanced-FT process, primarily due to the recycling loop. Thus, the IRR of the FT-advanced scenario was 9.1% higher, owing to reduced capital expenses and higher energy conversion and electricity export efficiency. As expected, the methanol scenarios that imported electricity to meet the steam utility deficits had the lowest capital costs at 279.4 and 293.1 million US$ for the conventional and advanced processes respectively, and therefore the highest IRR of 21.3% was obtained for the advanced methanol scenario that imported electricity. From a financial risk perspective, Fig. 6 shows that is no viability when comparing of the IRRs of the various processes against the minimum IRR of 25% required by private investors. Advanced methanol synthesis could however, be feasible for private investors when sugar mills run more efficiently, with steam economy at 0.36

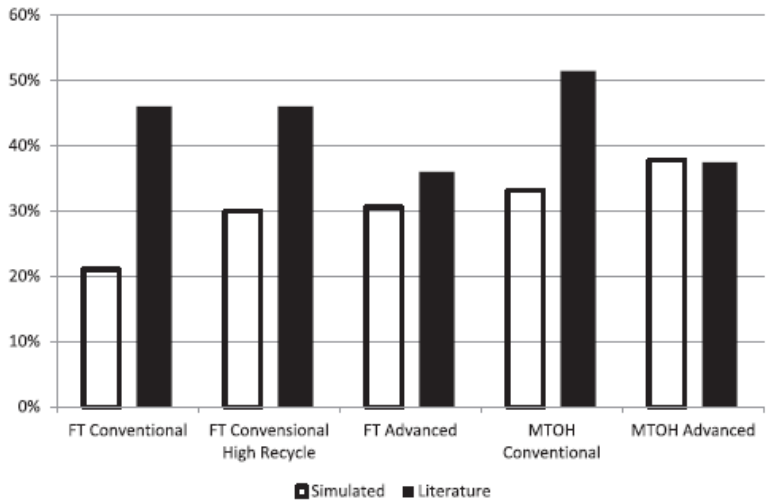


Fig. 5. Comparison of liquid yields determined for the simulation and from literature (FT conventional (Tijmensen et al., 2002); FT advanced (Larson et al., 2009); MTOH conventional (Hamelinck and Faaij, 2001); MTOH advanced (Hamelinck and Faaij, 2001)).

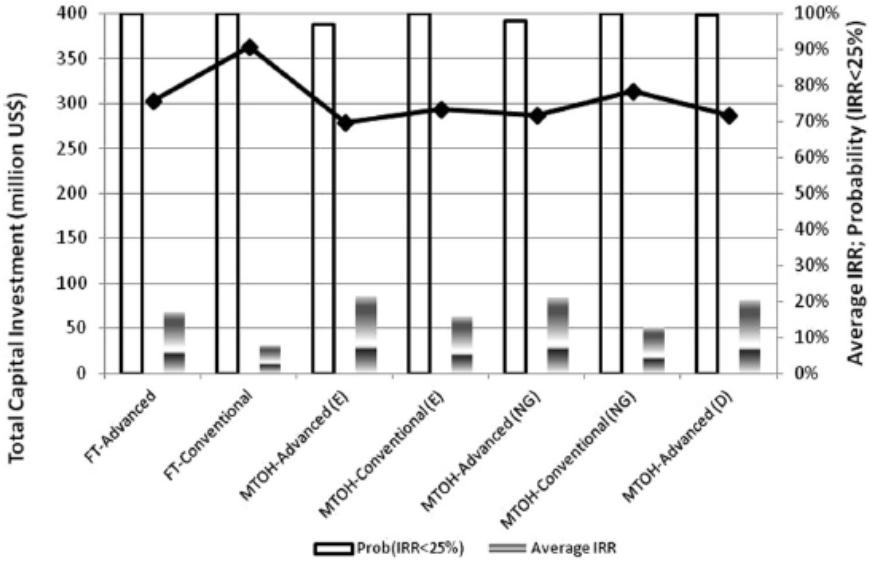


Fig. 6. Summary of economic indicators (FT – Fischer–Tropsch; MTOH – methanol synthesis; (E) electricity imports; (NG) natural gas imports; (D) diversion of syngas).

tonnes of steam per tonne of wet cane, which is a foreseeable target in the near future (Leibbrandt, 2010).

Importing natural gas to meet energy utility deficits increased the capital costs by 7.0% and 2.5% for the conventional and advanced methanol scenarios respectively, while simultaneously reduces the IRRs to 12.8% and 21.1%, respectively. The decrease in the IRR is due to the price of natural gas that is at 15.8 US$/GJ and therefore shows that the excess electricity exported from these scenarios could not offset the costs of natural gas. Comparing the cost of natural gas to the cost of production cost of syngas of 4.2 US$/GJ based on an allothermal gasification infers that the generation of the required steam and the excess electricity in the gas turbine using natural gas was more costlier.

The estimations of capital costs in the present simulations were compared to values reported by Larson et al., 2009 and Hamelinck and Faaij (2001) for synfuels production. For FT fuels production, this comparison was achieved by subtracting the capital costs for syncrude refining from the estimates provided by Larson et al., 2009, since the present study did not include economics of refining. The specific capital estimates for the advanced FT (255 US$/MJ HHV biomass input) and advanced methanol (235 US$/MJ) scenarios in the present study compared well to reported values for FT (266 US$/MJ after adjustment; (Larson et al., 2009)) and methanol (226 US$/MJ (Hamelinck and Faaij, 2001)).

3.3. Comparison with biological routes for bioethanol production through integration in RSI

The results of this study is compared with bio-ethanol production, where the hemicellulose fraction is used for ethanol production with the remaining fractions for power generation by Biomass Integrated Gasification and Combined Cycles (Petersen et al., 2014). The best efficiency for thermochemical production in this study was 37.7% for the advanced methanol scenario supplemented by natural gas, which competes favourably with the efficiency of biological scenario at 32.9% (Petersen et al., 2014). The most economically viable thermochemical process, which was the advanced methanol scenario that imported electricity, only obtained an IRR of 21.1%. The range of possible IRRs of the biological scenario, was between 29% and 35% depending on the pricing strategy (Petersen et al., 2014) that shows that the biological routes were much more lucrative from an economic perspective, even though the overall efficiencies of the thermochemical processes were higher.

Since the electricity and natural gas was only supplemented at respective rates of 1% and 4% of the total calorific input, it would not make any significant impact on the greenhouse gas reductions of the methanol product. While the biological scenario did not need any supplementation in terms of energy, it needed process chemicals that introduce greenhouse gas emissions into the life cycle.

4. Conclusion

Optimizing the syngas production from cane residues has showed that using allothermal gasification systems are preferable for integrating gasification-synthesis processes into the South African RSI. Techno-economic assessments have shown that methanol synthesis could not service the utility demands of the sugar mill, while FT synthesis could export excess electricity, with excessive steam. However, FT synthesis had lower economic viability as the advanced scenario had an IRR of 16.9% compared to 21.1% of the advanced methanol synthesis that imported electricity to satisfy overall energy demands. Overall, integrated thermochemical scenarios are currently not favourable for private investments.

Funding sources

The authors would like to thank the National Research Foundation of South Africa and the DBSA Green Fund Project for providing the bursary funds from which this research was conducted.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.biortech.2015.02.007.

References

Aspen Technology Inc., 2008. Aspen Plus®, Aspen Icarus®.
Baratieri, M., Baggio, P., Fiori, L., Grigiante, M., 2008. Biomass as an energy source: thermodynamic constraints on the performance of the conversion process. Bioresour. Technol. 99, 7063–7073.

Chen, C., Mathias, P.M., 2002. Applied thermodynamics for process modeling. AIChE J. 48 (2), 194–200.
Chen, P., Cheng, Y., Deng, S., Lin, X., Huang, G., Ruan, R., 2010. Untilization of almond residues. Int. J. Agric. Biol. Eng. 3 (4), 612–625.
Consonni, S., Katofsky, R.E., Larson, E.D., 2009. Chemical engineering research and design A gasification-based biorefinery for the pulp and paper industry. Chem. Eng. Res. Des. 7, 1293–1317.
Dijk, K.M. van et al., 1995. Methanol from natural gas: conceptual design & comparison of processes, Delft.
Dry, M.E., 2002. The Fischer–Tropsch process: 1950–2000. Catal. Today 71, 227–241.
Ekbom, T., Hjerpe, C. & Hermann, F., 2009. Pilot study of Bio-jet A-1 fuel production for Stockholm-Arlanda Airport, Stockholm.
Filippis, P.D., Borgianni, C., Paolucci, M., Pochetti, F., 2004. Gasification process of Cuban bagasse in a two-stage reactor. Biomass Bioenergy 27, 247–252.
Hamelinck, C.N., Faaij, A.P., 2001. Future Prospects for Production of Methanol and Hydrogen from Biomass. Utrecht University.
Holmgren, K.M., Berntsson, T., Andersson, E., Rydberg, T., 2012. System aspects of biomass gasification with methanol synthesis e Process concepts and energy analysis. Energy 45 (1), 817–828.
Jorapur, R., Rajvanshi, A.K., 1997. Sugarcane leaf-bagasse gasifiers for industrial heating applications. Biomass Bioenergy 13 (3), 141–146.
Kreutz, T.G., Larson, E.D., Liu, G. & Williams, R.H., 2008. Fischer–Tropsch fuels from coal and biomass. 25th Annual International Pittsburgh Coal Conference, (August).
Larson, E.D., Jin, H., Celik, F.E., 2009. Large-scale gasification-based coproduction of fuels and electricity from switchgrass. Biofuels, Bioprod. Biorefin. 3, 174–194.
Leibbrandt, N.H., 2010. Techno-Economics Study for Sugarcane Bagasse to Liquid Biofuels in South Africa: A Comparison between Biological and Thermochemical Process Routes (PhD Dissertation). Department of Process Engineering, University of Stellenbosch.
Leibbrandt, N.H., Aboyade, A.O., Knoetze, J.H., Görgens, J.F., 2013. Process efficiency of biofuel production via gasification and Fischer–Tropsch synthesis. Fuel 109, 484–492.
Macrelli, S., Mogensen, J., Zacchi, G., 2012. Techno-economic evaluation of 2nd generation bioethanol production from sugar cane bagasse and leaves integrated with the sugar-based ethanol process. Biotechnol. Biofuels 5, 1–18.
March, L., 1998. Introduction to Pinch, Linnhoff March LTD.
Morvay, Z.K., Gvozdenac, D.D., Morvay, Z.K., Gvozdenac, D.D., 2009. Part 3: toolboxes. In: Applied Industrial Energy and Environmental Management. John Wiley & Sons Ltd., pp. 1–34.
Ozkara-Aydınoglu, S., 2010. Thermodynamic equilibrium analysis of combined carbon dioxide reforming with steam reforming of methane to synthesis gas. Int. J. Hydrogen Energy 5 (1), 12821–12828.
Petersen, A.M., Aneke, M., Gorgens, J.F., 2014. Techno-economic comparison of ethanol and electricity coproduction schemes from sugarcane residues at existing sugar mills in Southern Africa. Biotechnol. Biofuels 7 (105), 1–19.
Pfeifer, C., Rauch, R., Hofbauer, H., 2004. In-bed catalytic tar reduction in a dual fluidized bed biomass steam gasifier. Ind. Eng. Chem. Res., 1634–1640
Phillips, S.D., Tarud, J.K., Biddy, M.J., Phillips, S.D., Tarud, J.K., Biddy, M.J., 2011. Gasoline from Wood via Integrated Gasification, Synthesis, and Methanol-to-Gasoline Technologies. National Renewable Energy Laboratory, CO.
Puig-arnavat, M., Bruno, J.C., Coronas, A., 2010. Review and analysis of biomass gasification models. Renew. Sustain. Energy Rev. 14 (9), 2841–2851.
Rapagna, S., Jand, N., Foscolo, P.U., 1998. Catalytic gasification of biomass to produce hydrogen rich gas. Int. J. Hydrogen Energy 23 (1), 551–557.
Richardson, J.W., Lemmer, W.J., Outlaw, J.L., 2007. Bio-ethanol production from wheat in the winter rainfall region of South Africa: a quantitative risk analysis. Int. Food Argibus. Manage. Rev. 10 (2), 181–204.
Richardson, J.W., Schumann, K. & Feldman, P., 2008. Simeter – simulation & econometrics to analyze risk.
Ryan, L., Campbell, N., 2012. Spreading the net: the multiple benefits of energy efficiency improvements. International Energy Agency, France.
Schuster, G., Lo er, G., Weigl, K., Hofbauer, H., 2001. Biomass steam gasi® cation ± an extensive parametric modeling study. Bioresour. Technol. 77, 71–79.
Silva, V., Rouboa, A., 2014. Optimizing the gasification operating conditions of forest residues by coupling a two-stage equilibrium model with a response surface methodology. Fuel Process. Technol. 122, 163–169.
Sims, R.E.H., Mabee, W., Saddler, J.N., Taylor, M., 2010. An overview of second generation biofuel technologies. Bioresour. Technol. 101 (6), 1570–1580.
Sun, L., Smith, R., 2013. Rectisol wash process simulation and analysis. J. Clean. Prod. 39, 321–328.
The Institute of Electrical and Electronics Engineers Inc., 2002. Power System Economics Designing Markets for Electricity, John Wiley & Sons Ltd.
Tijmensen, M.J., Faaij, A.P., Hamelinck, C., Van Hardeveld, M.R.M., 2002. Exploration of the possibilities for production of Fischer Tropsch liquids and power via biomass gasification. Biomass Bioenergy 23, 129–152.
Wienese, A., 2001. Boilers, boiler fuel and boiler efficiency. In Proceedings: The South African Sugar Technologists' Association 75, 275–281.

CHAPTER 7: Integration of Combined Synthetic Fuels and Bioethanol Processes at Sulphite Mills

Title of Article to be written: "Assessing the Technical, Economic and Greenhouse Gas Reduction Potential of Combining Ethanol and Synthetic Fuel Production Scenarios at Sulphite Pulping Mills"

Contribution of this Chapter

In this chapter, the potential of combining synthetic fuel and bioethanol production at a sulphite mill was explored, to arrive at a process with high liquid yields and improved economic performance. Details regarding the rate of residue generation and their chemical characteristics found in Chapter 5 formed the basis of this study. Flow sheet designs in this chapter adopted as a basis the most feasible process scheme for ethanol production from SSL, as described in Chapter 5, while the heat and power generation via direct combustion flow-sheet, as described in Chapter 5, was replaced by (i) a Biomass Integrated Gasification and Combined Cycles as developed in Chapter 4, (ii) advanced methanol synthesis or (iii) Fischer-Tropsch process flow sheets, as developed in Chapter 6. For replacements ii and iii, the method for optimising syngas production developed on Chapter 6 was adapted for producing syngas from bark in the pulp and paper industrial environment.

In terms of the overall objectives of this dissertation, it was shown that feasible scenarios for combined synthesis fuels and bioethanol are possible at Sulphite pulp-mills. In terms of the objectives relating to the applications of flow-sheet analysis, it was shown that negating disposal costs by using waste biomass for synthesis processes to enhance the yield of valuable products where ethanol is produced from SSL enabled economic feasibility at small scales.

Authors' contributions

Abdul Petersen is the primary author and investigator of the research in this chapter. JFG is the study group leader and approved the paper as a formal submission from the research group. All the authors read manuscript and approved the integrity and accuracy of the results presented.

Assessing the Technical, Economic and Greenhouse Gas Reduction Potential of Co-locating Ethanol and Synthetic Fuel Production Scenarios at Sulphite Pulping Mills

1 Introduction

The flow-sheet analysis of biofuel production concepts in the Paper and Pulp Industry (P&PI) has focussed primarily on the Kraft Process[1–4], even though ethanol generation from residues in the Sulphite Processes is already an industrial practice[5]. Previous flow-sheet analysis studies have explored biological process routes to convert residual sugars in a substrate (such as Spent Sulphite Liquor) to ethanol (Chapter 5[6] and Magdzinski[5]), or the thermochemical chemical conversion of Black Liquor (BL) or other forestry wastes to synthetic fuels[1–3]. In either case, the fuel production process from pulp and paper residues resulted in a deficit in meeting the energy requirements of the P&PI facility, since these residues are typically used to generate a portion of the heat and power utilities[7,8]. Furthermore, the energy requirement of the biological fuel production process compounds the deficit in the energy generated from the residues, creating a greater reliance of the adjacent pulping facility on supplementary energy sources [4,8].

Synthetic fuel production through the thermochemical gasification-synthesis process has focused primarily on the conversion of BL to synthesis gas (syngas) with the Chemrec Technology™ (with some recent developments in sodium based Sulphite Processes[9]), which entails a high pressure entrained flow gasifier with a chemical recovery quench, followed by a heat recovery system and acid gas removal process[1–3]. The syngas is then used to synthesise liquid fuels, such as Fischer-Tropsch fuels or methanol, and the un-reacted gasses are then used to generate heat and

power (utility energy), integrated into the energy supply of the P&PI facility. In some cases, only the conversion of forestry residues to fuels by gasification-synthesis has been considered, while integrating the excess heat and power generated to an existing pulp mill[10]. Other studies have sought to improve the production of liquid fuels and utility energy, by incorporating bark and hog-fuel as supplementary fuels for syngas production in a pressurised gasifier[3] in addition to BL gasification. While pressurised gasification systems avoid the costs associated with downstream syngas compression[11], the overall costs of syngas generation using allothermal gasification has shown to be much lower, in the context of integrating synthetic fuel processes in the Raw Sugar Industry (Chapter 6[12]).

Studies on ethanol production at Kraft Processes have explored the possibility of extracting hemicellulose from lignocellulose prior to Kraft pulping, in order to convert the hemicellulose to ethanol via fermentation[4,8]. Regarding the Sulphite Process based on hardwood processing, optimising ethanol production from the SSL that is dominated by pentose sugars has been successful on a laboratory scale[13,14], while flow-sheet analysis for industrial application has shown that economic viability is largely dependent on the strategy for integrating the ethanol fermentation and the energy utilities required for distillation (Chapter 5). The implication on the energy balance resulting from ethanol production was twofold, since the calorific content that would otherwise power a boiler is reduced and because of the energy duties for the ethanol purification. For either the Kraft and Sulphite scenarios however, the net utility energy increase from integrating ethanol production is fulfilled by supplementing the boiler with alternative fuel sources such as bark (Chapter 5[6] and other literature[8]). From the perspective of a life cycle assessment, the supplementary fuel must be from a renewable source (such as bark or other forestry residues), otherwise there is no net reduction in global warming potential (GWP) associated with the ethanol production, such as when coal is used as the supplementary fuel (Chapter 5).

It was shown in Chapter 5 that the optimal configuration for ethanol from SSL (30% solids concentration in SSL, atmospheric distillation) had a net steam and electricity requirement of 0.10

tons and 35.75 MJ per cubic meter (m^3) of SSL converted to ethanol, and bark was available at a rate of 0.06 tons per m^3 of SSL. For the gasification-synthesis process it was shown in Chapter 6 that the yields of surplus steam and electricity were 1.71-2.72 tons and 709-1418 MJ per ton of lignocellulosic biomass, respectively, for synthesis of intermediate synfuels like bio-methanol and bio-syncrude. Thus, it is possible to improve the liquid fuel yield at Sulphite mills by combining the SSL conversion to ethanol at with the synfuels production by gasification-synthesis from bark, which would then also provide steam and electricity from the exothermic heat[15]. The surplus of steam and electricity from the bark gasification-synthesis process would be sufficient to meet the total energy utility demands of the combined facility, where SSL-ethanol production is integrated into the Sulphite mill. The production of intermediate synthetic fuels is preferred to final synfuels such as Fischer Tropsch (FT) gasoline due to less capital intensive production costs [16], which, combined with the avoided costs of bark disposal, can provide economically viable synfuels production at small scales[17].

The aim of this chapter is to assess the technical, economic and net greenhouse gas reduction potential (NGGRP) for combining bio-synthetic fuels (methanol or FT-syncrude) synthesis with the production of ethanol from SSL, as combined integrated scenarios into a Sulphite mill. The surplus energy utilities generated by the gasification-synthesis processes should satisfy the net energy demands of the combined ethanol production and sulphite mill. The gasification-synthesis processes developed in Chapter 6[12] will be adapted for converting bark to syngas, by adjusting the optimising procedure for integrating biomass gasification in a facility representative of the P&PI, rather than that of the Raw Sugar Industry (RSI). The outcomes of the various co-locating scenarios will be compared against the outcomes of Chapter 5, where the bark residues are converted to energy via combustion processes, and modified heat and power scenarios, such as Biomass Integrated Gasification and Combined Cycles (BIGCC)[18]. The potential contribution of alternative energy supplementation processes, such as the biodigestion of Sulphite mill effluent, will also be investigated.

2 Overview of Process Technologies

In this section, an overview of the simulations and outcomes of process technologies developed for the integration of biofuel production into industries such as the RSI (Chapter 4 and 6) and Sulphite Pulping Mill (Chapter 5) is given. From this overview, the most suitable of the process technologies considered in the previous chapters, can be selected for the present co-location scenarios.

2.1 Ethanol Production from Magnesium Oxide Spent Sulphite Liquor (Mg-SSL)

The optimal ethanol flow sheet configuration developed in Chapter 5 (see Figure 14) consisted of diverting the partially-concentrated Mg-SSL at 30% solids content from the multi-effect evaporation train, which concentrates SSL from an initial concentration of 10% to about 60% for fuelling a ANDRITZ Recovery Boiler system [19]. The required concentration of 30% was achieved after the 5th effect, and therefore, the SSL was diverted at this point for further processing to produce ethanol. Initially, it was detoxified to improve its potential to be fermented, and thereafter, a portion was split-off for yeast propagation, while the remainder is applied for ethanol fermentation. The fermentation broth was then subjected to conventional atmospheric distillation to produce anhydrous ethanol that is purified with molecular sieves. The distillation residue from the beer column was then returned to the last effect in the evaporation series to increase the solids concentration in the syrup to 55-60%, which is the level required for the recovery boiler. The recovery boiler raised steam at 49 bar, which was then expanded to 8 bar, and used as the live steam supply.

Chapter 5 also considered a combined heat and power (CHP) generation system using bark for the SSL-ethanol process that entailed a Combustion- High Pressure Steam (CHPS) System that had risen steam at 85bar[20] that was expanded to 49 bar, and then to 8 bar to serve as live steam

supply to the plant. The CHP system generated energy utilities in excess of the net requirements of the ethanol production, and the excesses were used to displace an equivalent amount of coal that is used in the Sulphite process.

2.2 ADVANCED POWER GENERATION FROM BARK

As an alternative to the CHPS system described in Chapter 4, the production of heat and power using BIGCC technology is also considered. This technology, which was described in Chapter 4[18], consists of an air-blown, fluidised bed gasifier, to produce product gas that is subsequently reformed and scrubbed[21,22]. The cleaned product gas is then compressed for combustion in the gas turbine, and the heat is recovered from the steam with a Heat Recovery Steam Generator (HRSG) to produce steam at 60 bar, which is then expanded for utility steam. It is an efficient and economical viable method of generating utilities for ethanol production, especially when combined with multi-effect distillation for ethanol purification (Chapter 4[18]). This synergy occurs because multi-effect distillation is primarily electrically driven and saves on stream consumption, while BIGCC technology produces electricity with high efficiency, but is restricted in its capacity for steam generation.

2.3 GASIFICATION-SYNTHESIS FOR SYNFUELS PRODUCTION

2.3.1 Syngas Production from Biomass

In chapter 6, an optimal flow sheet configuration for producing syngas from lignocellulosic biomass was determined, using Aspen Plus® simulations. Optimum gasification parameters (moisture content, equivalence ratio or biomass split and steam-to-biomass) were determined for a system to convert lignocellulose to cleaned syngas in a cost effective and efficient manner. The effects of these parameters on all the system components, which included biomass drying, oxygen production via an Air Separation Unit (autothermal), gasification, combustion for heating a transfer

medium (allothermal), steam production from syngas via a Heat Recovery Steam Generator, syngas compression and acid gas removal were considered. Comparing three alternative syngas production systems optimised in this manner showed that catalytic allothermal gasification was preferred due to the lower cost of producing cleaned, compressed syngas at an acceptable efficiency.

2.3.2 Methanol Synthesis

In Chapter 6, processes for integrating methanol synthesis (MTS) following optimal syngas production for into a RSI facility were configured. It was shown that the advanced synthesis technology was advantageous in all respects, since it produced a higher liquid yield and consumed less energy utilities, allowing a greater potential for integrating purposes. Capital costs were less for the advanced system and the IRRs were up to 2.1 times more than that of the conventional technologies.

2.3.3 FT bio-syncrude Synthesis

Conventional and advanced systems for FT synthesis of bio-syncrude were also considered and the advanced FT synthesis was shown to have higher liquid yields, while the conventional system produced more electricity to be sold to the grid. From an economic perspective, the conventional system did not have any viability because of the high capital expenditure and low yield of valuable product. The IRR of the advanced system were about double that of the conventional system.

3 Methodology

3.1 PROCESS DESCRIPTIONS

3.1.1 Baseline models: Ethanol Production and Heat and Power Generation from bark using Combustion

The detailed process description for ethanol production from Mg-SSL concentrated at 30%, as well as the conversion of bark to heat and power is given in Chapter 5. The chemical compositions of these residues are also given in Chapter 5 and the respective flow rates for SSL concentrated at 30% is 95.94 tons per hour and that of the bark is 34.00 tons per hour. A detailed process flow diagram for these processes that also summarises the modelling parameters is depicted in Figure 14.

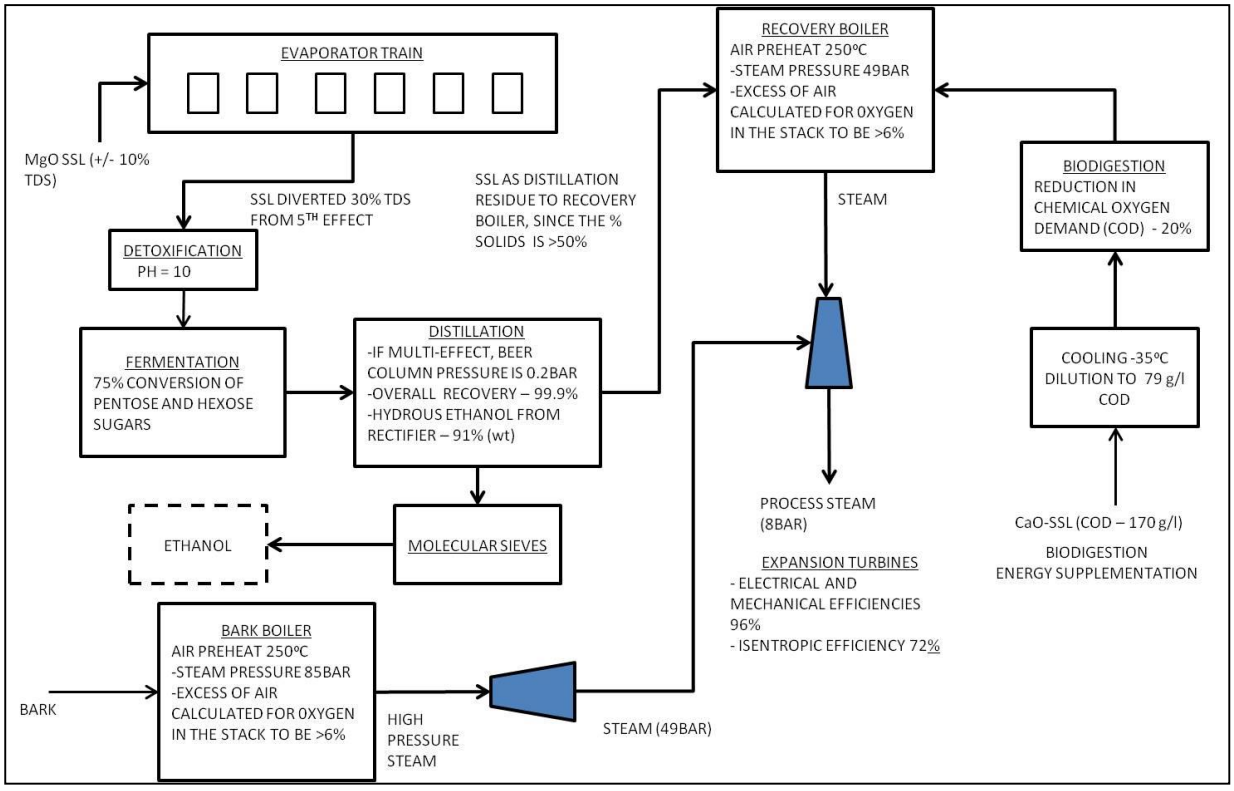


Figure 14: Baseline Ethanol Production; Conversion of Bark to Heat and Power, Energy Supplementation from Biogas

3.1.2 Energy Supplementation from biodigestion

The scenarios described in Chapter 5 for SSL-ethanol production will be expanded in the present chapter to include to potential contribution of a biodigestion facility for energy supplementation. This scheme was also modelled in Chapter 5 using the portion of the SSL coming from the calcium oxide based digestion line that is discharged as effluent (flow rate = 85.5ton/hr) in a USAB biodigester to generate biogas that supplement the recovery boiler, using the experimental data of Jantsch et al[23].

3.1.3 Advanced Heat and Power Generation Using BIGCC

The process for converting biomass to heat and power with BIGCC technology is described in detail in Chapter 4[18]. A detailed process flow diagram that also summarises the technical inputs is shown in Figure 15.

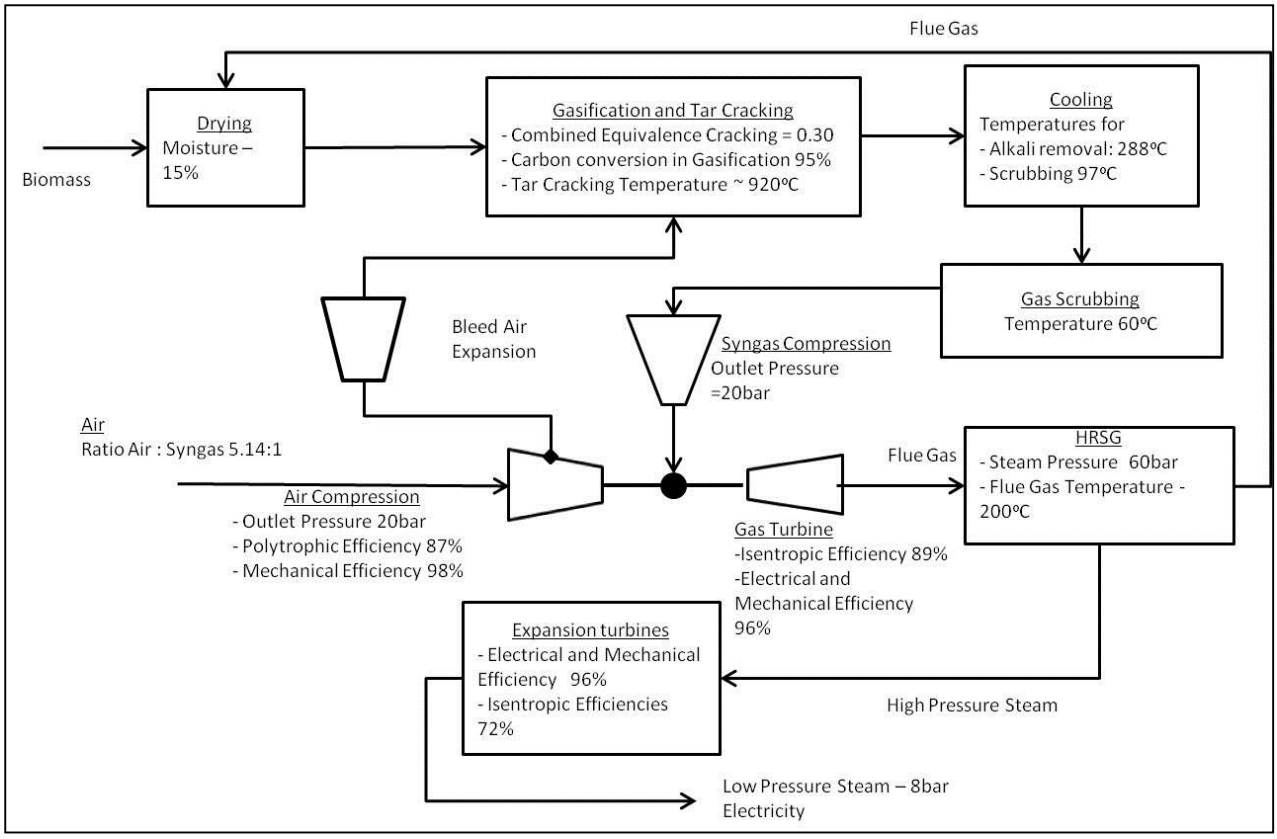


Figure 15: Conversion of Bark to Heat and Power by BIGCC technology

3.1.4 Co-location of Gasification-Synthesis with SSL-ethanol Production

A. Optimisation of Syngas Production

The procedure for optimising the production of syngas from bagasse and trash in terms of conversion efficiency (CE) and overall costs, described in Chapter 6, is adapted for the P&PI in the present chapter, using bark as feedstock. The cost of syngas production (CSP) was quantified as the amortised capital cost (AMC) and the operating opportunity cost (OOC), and it is the OOC that requires adaptation to reflect the interaction of steam and electrical utilities between the production of syngas and the energy supply system of the Sulphite mill. In Chapter 5, this interaction was defined by the equivalent amount of coal needed to generate the shortfall in steam and electricity demands of the integrated

ethanol-sulphite process, and is therefore adapted here to mean the amount of coal needed to generate the requirements of syngas production. Therefore, the OOC is defined as the cost of the additional coal for generating the steam and electricity that the production of clean-compressed syngas entails; and since the production of syngas can result in a net generation of these utilities, the OOC can obtain a negative value.

Determining the relationship between the quantity of coal needed to generate high pressure (HP) steam, low pressure (LP) steam and electricity required a simulation of a CHP in Aspen Plus®. Coal is combusted to raise high pressure steam, of which utility demands are firstly withdrawn, with the remaining expanded to the low pressure utility steam at 8bar. To generate the data needed to relate coal flow rates to electricity and steam generated, the Sensitivity Analysis feature of Aspen Plus® was employed to vary the coal flow rate. The data generated was then regressed as linear equations shown by Equations 1 and 2 and the expression for the CSP is given in Equation 3. (Note: In Equation 3, the maximum requirement of coal between the LP steam and electricity is considered, as these utilities are generated from the same steam line. Thus, if the electricity demand required more coal, then the steam generated by that amount of coal would be in excess of the syngas steam demand.)

$$Electricity = Coal * 1.109 - 0.017 \quad (1)$$

$$Steam = Coal * 6.863 + 0.021 \quad (2)$$

$$\text{CSP} = \frac{(\text{Coal}(\text{HP}_{\text{SBR}} - \text{HP}_{\text{Generated}}) + \text{Maximum}(\text{Coal}(\text{Electrity}); \text{Coal}(\text{LP})) * \text{Coal\_Price} + \text{AMC}}{\text{Syngas Chemical Energy}} \quad (3)$$

Where HP – high pressure steam; SBR – steam to biomass ratio; LP – low pressure steam; AMC – amortised capital cost; Coal_Price – 115.8 US$.ton

Thus, for the optimisation of the syngas production, the CSP was minimised while the CE was maximised, subjected to the constraints that the molar H2:CO ratio was 2 and the temperature was greater than 900^{o}C, using the methodology described in Chapter 6. The two systems considered for optimisation was the pressurised autothermal (Figure 16A) and atmospheric allothermal (Figure 16B) gasification.

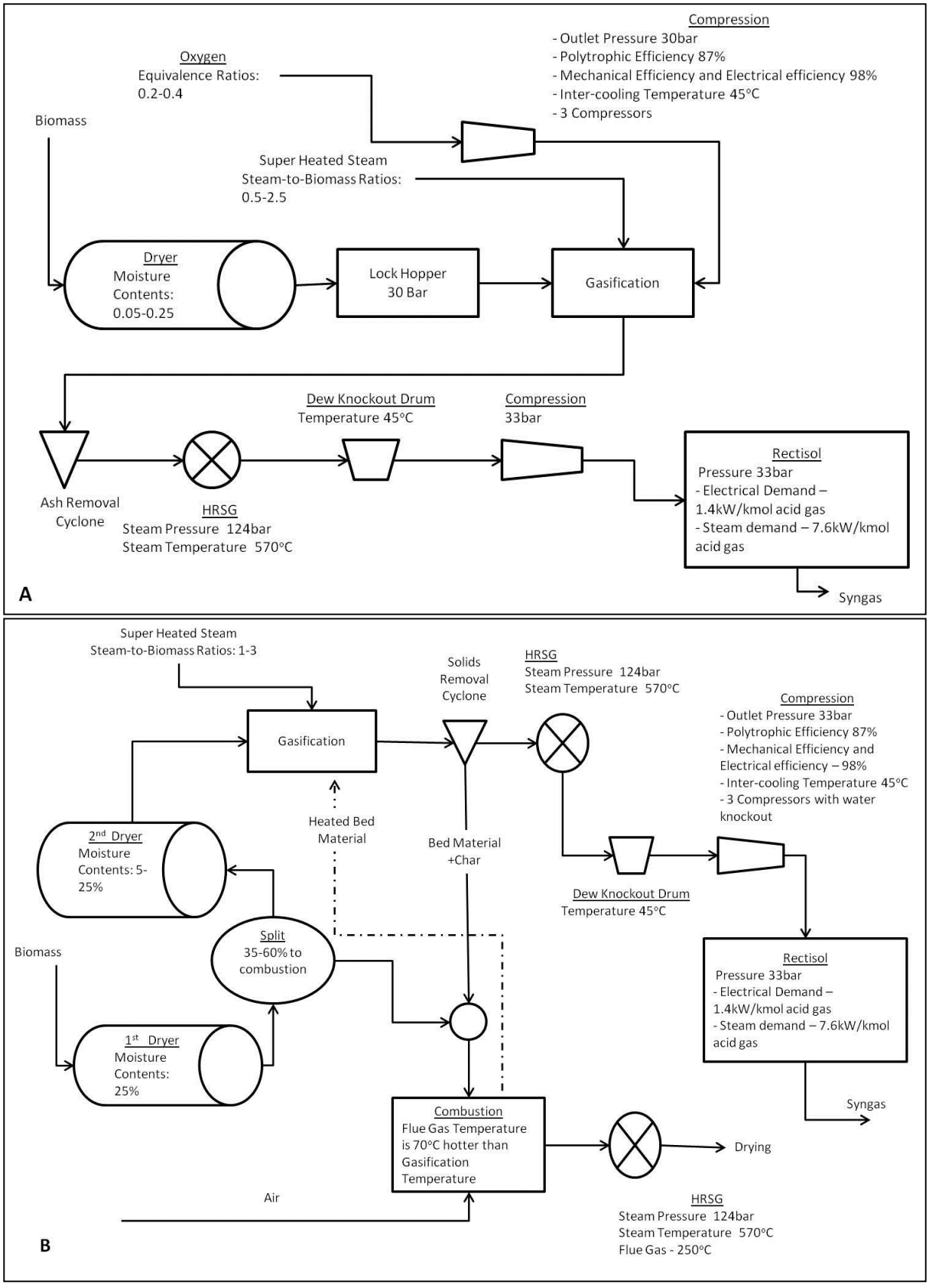


Figure 16: Production of Syngas from bark using A) Pressurised Autothermal and B) Atmospheric Allothermal Gasification

B. Synthetic Fuel Processes

The advanced liquid phase reactors were preferred for synthesis of both FT syncrude and methanol from syngas, as described in Chapter 6. The process flow diagrams that detail the process and unit parameters are shown in Figure 17 for methanol synthesis and Figure 18 for FT synthesis.

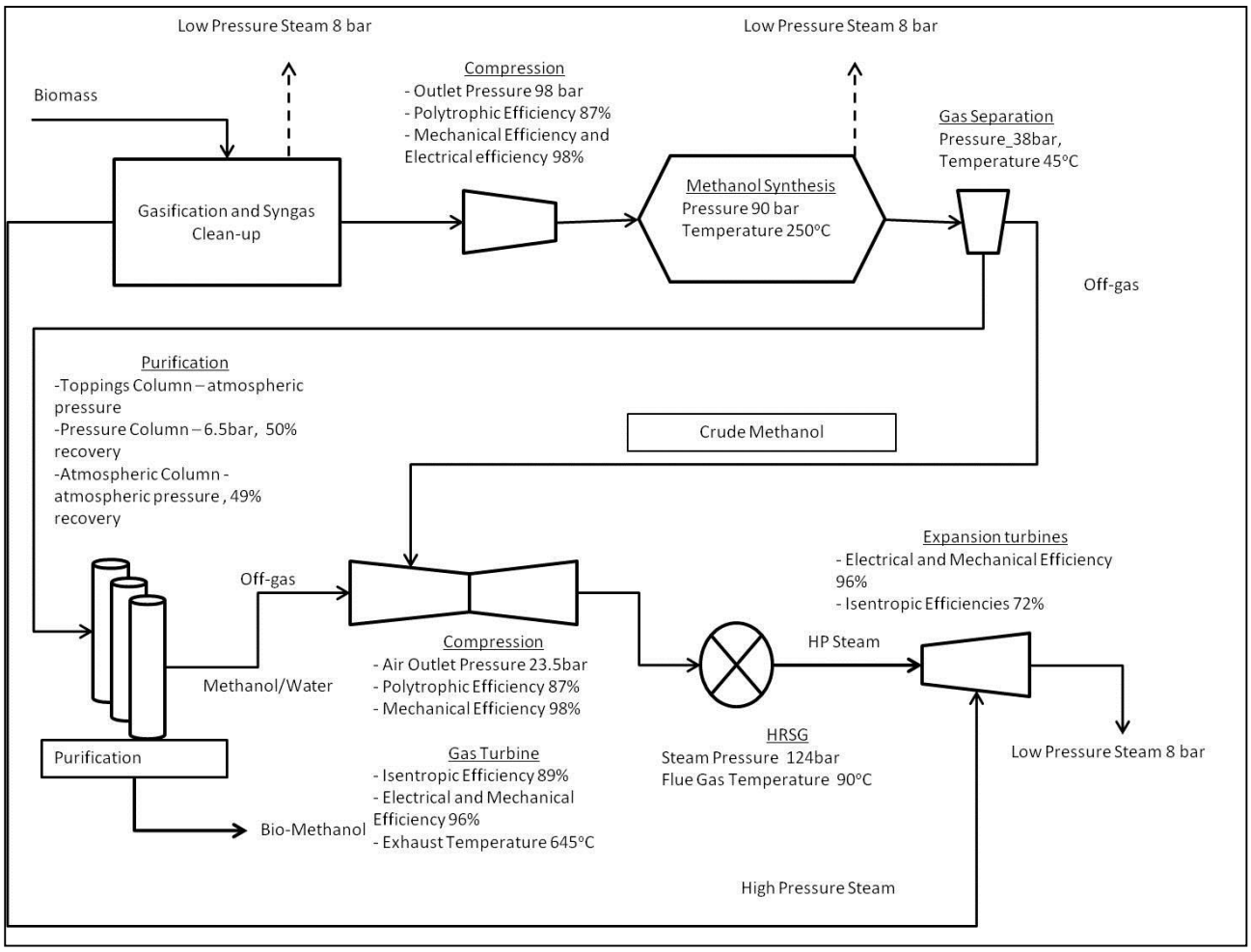


Figure 17: Methanol Synthesis using advanced liquid-phase reactor technology

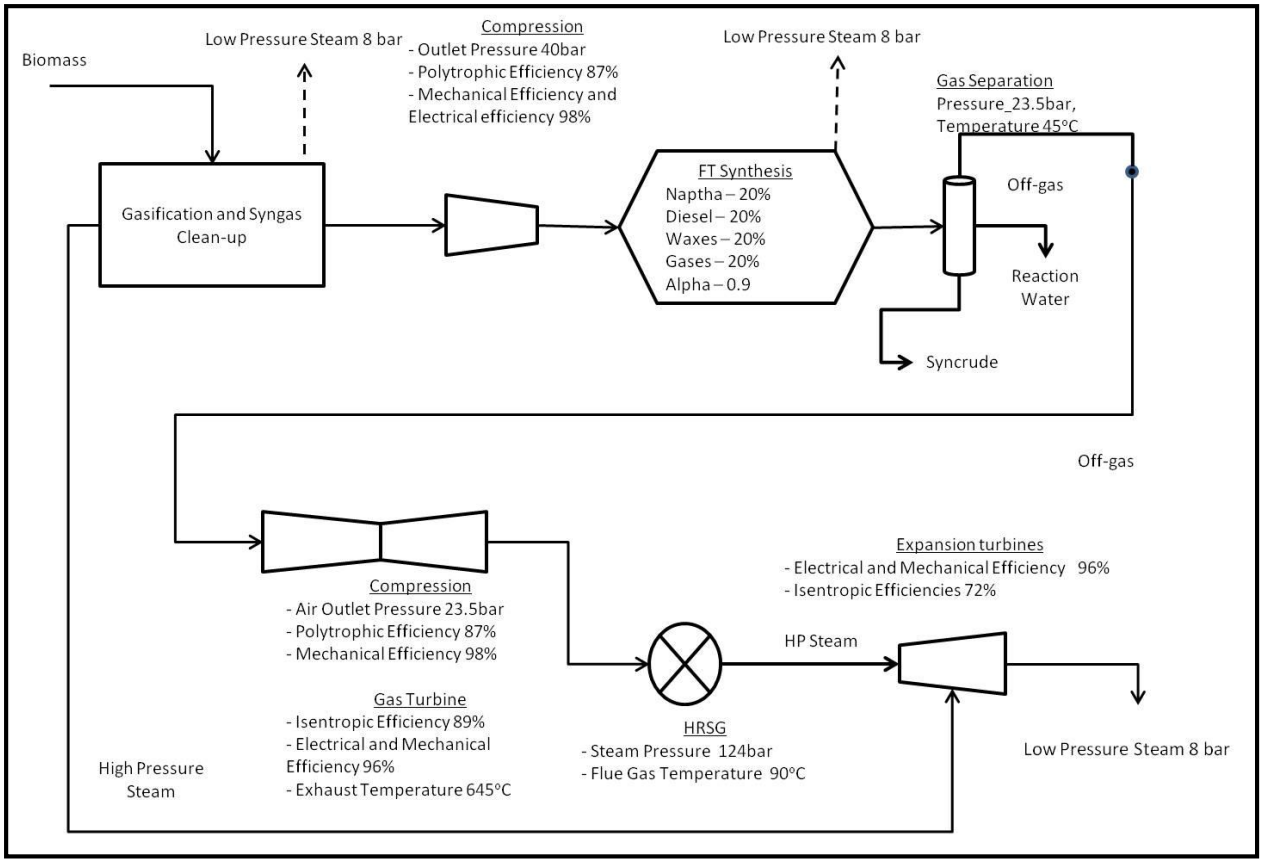


Figure 18: FT Synthesis using Slurry Phase Reactor Technology

C. Power Utilities and Heat Integration

The generation of heat and power from off-gases after the synthesis processes, using gas turbines and HRSGs, described in Chapter 6, are shown in Figure 17 and Figure 18 for methanol and FT synthesis respectively. The high pressure steam generated from the HRSG is combined with that generated by syngas production and expanded to 8 bar, which is then returned to the Sulphite mill as live steam. Low pressure steam at 8 bar was generated from the waste heats of the gasification-synthesis process, where the temperature was high enough, such as the FT and Methanol reactor. Waste-heat from low temperature processes was discarded in a cooling tower, as described in Chapter 6.

3.1.5 Relating power utilities to the equivalent amount of coal of the Integrated Ethanol-Sulphite Process

In Chapter 5, the amount of coal needed to satisfy the steam or electricity demands of the various ethanol scenarios was determined, using correlations formulated from Aspen Plus® simulation of a coal-fired CHP plant ran using the Sensitivity Analysis tool to relate the rate of coal consumption to the rate of utility generation. The relationships established was STEAM=7.249*COAL+0.008 and ELECTRICITY=0.755*COAL-0.021, which are reflective of the current energy circuit that generates steam at 49 bar, which is then expanded to 8 bar. These relationships differ from the relationships used for syngas productions, as those determined the amount of coal needed to supplement the generation of high pressure steam at 124 bar in the synthesis processes[24].

3.2 DEFINITIONS OF SCENARIOS DEVELOPED

The process scenarios created by the various combination of the sub-process described is named and abbreviated in Table 10.

Table 10: Process Scenario Descriptions

30%-ME-BTE	Ethanol produced from SSL concentrated at 30%, with multi-effect distillation, with direct conversion of bark to heat and power
30-ME-BIGCC	Ethanol produced from SSL concentrated at 30%, with multi-effect distillation, with conversion of bark to heat and power by BIGCC
30%-CON-BTE	Ethanol produced from SSL concentrated at 30%, with conventional distillation, with direct conversion of bark to heat and power
30%-CON-MTS	Ethanol produced from SSL concentrated at 30%, with conventional distillation, combined with methanol synthesis from bark
30-CON-FT	Ethanol produced from SSL concentrated at 30%, with conventional distillation, combined with FT crude synthesis from bark
--**-BG	Scenario considering energy supplementation with biodigestion of effluent

3.3 NET GREENHOUSE GAS REDUCTION POTENTIAL

In chapter 5, the NGGRP of processing scenarios were calculated using life cycle techniques, based on the $CO_{2(eq)}$ emissions of all stages included. The boundary defined in Chapter 5 will apply here, which encapsulated all stages involved from the SSL generation to the ethanol fuel consumption, including the emissions associated with the chemicals used[25]. The boundary includes the emissions associated with the additional coal needed if the utilities generated by the synthesis or biomass-to-energy processes did not fulfil the requirement of net utility increase of the integrated ethanol-sulphite mill or otherwise, the emissions avoided by the coal displaced by utilities generated in excess. The boundary extends to include the displacement of emissions associated with the fossil derived fuel by the use of biofuel products produced[26,27]. Thus, ethanol displaced the gasoline on an energy equivalent basis, while the emissions associated with fossil derived gasoline and diesel was displaced with the equivalent derived from bio-syncrude[28]. With regards to bio-methanol, it either displaced the emissions of gasoline directly on an energy equivalent basis or the emissions associated with the fossil derived methanol that used in biodiesel[25]. The placement of the overall boundary is reflective of the "Consequential-type Life Cycle Analysis", which quantifies the effects of the processes involved in a technological alteration and variations[29].

The avoided emissions associated with FT bio-syncrude was calculated by assuming that the product distribution of gasoline and diesel is 33% and 67% on a calorific basis[24], and a crude oil refining efficiency of 94.4%[30]. Thus, after taking the crude refining efficiency into account, the total amount of greenhouse gas emissions displaced by 1 litre of bio-syncrude was 2.21 was kg CO_2(eq) based on the specific emissions of 2.35 and 2.34 kg CO_2(eq) from gasoline and diesel, respectively (numbers recorded from GREET 8.1[31] database). For the calculation of emissions

avoided by replacing the fossil derived methanol in biodiesel, the basis was the value of the total CO_2(eq) in the GREET 8.1[31] database, emitted from an engine combusting 1 litre of Biodiesel 20. This blend consists of a 80:20 ratio of diesel to biodiesel by volume. The carbon balance of biodiesel derived from extracted oils can typically have a fossil carbon content of 43.3% in its life cycle and methanol constitutes 22.1%[32] of this. Thus, the contribution of methanol to the total CO2 (eq) emission of 1 litre of biodiesel combusted is 0.23 kg. This translates to a displacement of 1.56 kg of $CO2_{(eq)}$ per litre of bio-methanol produced. Otherwise, the alternative method used to account for emissions displaced by biomethanol was that it would be blended into gasoline, and that the reductions would be proportional to the energy equivalents.

3.4 ECONOMIC EVALUATION

In order to be consistent with the modes of economic analysis carried out in Chapters 4,5 and 6; Monte Carlo based methods for a Financial Risk Assessment (FRA) were applied here as well[33–35]. This was done to quantify the risk associated with an investment that is deduced from a probability distribution generated for the key economic indicator, the Internal Rate of Return (IRR). The probability distribution was generated by accounting for the historical fluctuations in the inputs of key economic parameters, such as the commodity prices, interest and inflation indices. The procedure adopted for carrying out the FRA is detailed in the Support Information Files for Chapters 5 and 6.

The estimation of the capital costs for all scenarios was based on estimates found in literature for the major equipment and Aspen Icarus® for the minor equipment, as detailed in the Support Information Files for Chapters 4 and 5. The total installed capital costs included all major, minor equipment, installation costs and the Balance of Plant (BOP) costs. The total investment costs then factored in additional costs contingency and site development. The methods and data used for estimating capital costs are also presented in the support information files for Chapters 5 and 6. It

must be noted in the capital estimation of co-location scenarios, the total equipment costs was the combination of those for synthesis fuels and ethanol production.

4 Results and Discussion

4.1 Optimisation of Syngas Production

The comparison between pressurised autothermal gasification (AUT_G(P)) and atmospheric allothermal (ALO-G) gasification for syngas production from bark is shown in Table 11. While the efficiency of the AUT_G(P) was 14% higher than the ALO-G, the total syngas production cost was about 64% more, making ALO-G the preferable model of gasification for the co-locating of synthesis fuels generation from bark with ethanol production at a Sulphite pulp mill. As shown in Chapter 6, the high costs associated with the pressurised gasification results from oxygen production and the capital costs associated with the pressurised gasification system. A possible implication is that the overall costs of synthesis fuels in Consonni et al[3] could have been lower had allothermal based systems been used instead of pressurised gasification, which would have resulted in a slightly lower fuel yield.

Table 11: Syngas optimisation

Mode of Syngas Generation	*UNITS*	*AUT-G(P)*	*ALO-G*
Specific Costs	(US$/GJ)	5.64	3.43
H2/CO		1.85	1.99
Gasification Temperature	^{o}C	1000	908.38
Conversion Efficiency		80.56%	71.52%

When comparing against the cane residues in Chapter 6, bark had the greater calorific value of 17.9 MJ/kg$_{(LHV)}$ when compared to that of the cane residues at 16.3 MJ/kg$_{(LHV)}$ (calorific values

calculated with the correlation of Channiwala and Parikh[36]), due to the lower oxygen content of bark. Thus, the gasification conditions of bark were generally more intensive in terms of the oxidation requirement and the equilibrium temperature obtained for the pressurised gasification of bark was 1000^{o}C, compared to 881^{o}C for cane. Thus, as the higher temperature of the syngas would allow a greater generation of high pressure steam to offset production costs during pressurised autothermal gasification with bark, it would also lower the conversion efficiency as more oxidation occurs. Thus, when cane residues were considered for syngas productions, the cost for the pressurised system was 80% higher than the allothermal system, which is higher than the difference considered in the context where bark is gasified where the difference is 64% since. Furthermore, the difference in efficiency between pressurised autothermal and allothermal was 12.21 %points with cane compared to 9.04% with bark.

4.2 TECHNO-ECONOMIC OUTCOMES

The technical outcomes in terms of the fuel output, net utility demands of the integrated ethanol-sulphite process, fuel output and power utilities generated by thermochemical process and power utilities generated by the exclusive heat and power producing system is shown Table 12. The amount of coal that was displaced or subsequently required and the NGGRP for all processes is shown in Table 12. With methanol and FT syncrude co-location with the integrated ethanol production in a Sulphite mill increased the total fuel production by 4.9 and 4.2-fold, respectively, compared to ethanol production alone, on a calorific basis. The yield of methanol is generally expected to be higher than that of syncrude, since methanol synthesis reactions do not produce oxidation products, such as H_2O in the case of FT synthesis. Subsequently, the generation of steam generated from the unconverted syngas as well as the steam generated as process heat by methanol synthesis could not satisfy the net energy demand of the integrated ethanol-sulphite mill. Thus, co-locating methanol required an additional coal supply of 0.007MJ per MJ of the total fuel produced, to satisfy the energy demands of the adjacent ethanol-sulphite mill.

Table 12: Fuel output, net utility demands of ethanol and supply; coal demand and displacements; greenhouse gas reduction potentials of co-location scenarios (Conversion to heat and power via combustion BTE, and BIGCC; FTS – Fischer Tropsch Synthesis, MTS – methanol synthesis)

Ethanol Scenario	Conventional			Multi-effect	
Thermochemical Scenario/Power Production	**BTE**	**FTS**	**MTS**	**BTE**	**BIGCC**
Net Outputs					
Bioethanol Production (l/hr)	2321	2321	2321	2321	2321
Thermochemical Fuel Production (l/hr)		3796	9366		
Total Liquid Product Output (MW_{th} HHV)	15.09	63.11	74.63	15.09	15.09
Ethanol Utility Demand					
Total Additional Steam Utility Required	29.56	29.56	29.56	19.82	19.82
Total Additional Electricity Utility Required	2.83	2.83	2.83	4.63	4.63
Return Utility Supply from Thermochemical Processes					
Steam Supply (tons/hr)	75.80	49.68	27.53	75.80	58.70
Electricity Generation (MW)	10.57	4.07	2.20	10.57	27.13
Displacement of Coal (tons/hr)	-6.38	-1.64	0.85	-7.72	-5.20
Utility Causing Maximum Coal Displacement	Steam	Steam	Steam	Electricity	Steam
Greenhouse Gas Reductions (tons/per)	20344	14627	13329 (± 0.7%)	24353	16844
Biodigestion - BTE Schemes					
Displacement of Coal (tons/hr)	-7.44	-2.41	0.07	-8.63	-6.43
CO2 Savings (tons/hr)	23524	16935	15637 (±0.6%)	27070	20512

A further comparison of the co-location of synthesis fuels scenarios shows that methanol synthesis had the higher fuel yield, but FT synthesis had a higher NGGRP. This is a result of the FT syncrude having the potential to offset 1.5 times more CO_2(eq) per litre of product than methanol. Additionally, the power utilities that FT synthesis generated had caused a displacement in the coal requirement of the ethanol-sulphite processes; whereas the integrated ethanol-sulphite processes demanded more coal when co-located with methanol synthesis, even with the supplementation of

energy from the biodigestion of the Ca-SSL. Table 12 also shows that the variation in the NGGRP associated with bio-methanol by altering its final use as a fuel ranges from 0.7 to 0.6% (showed in parenthesis), which implies that there is no appreciable difference in the NGGRP between using methanol as an intermediate fuel carrier or when substituting gasoline directly.

In order to determine whether the performance of exclusive power generation can be enhanced by an advanced technology, the ethanol production scenario that used multi-effect distillation and a BIGCC system for heat and power generation was assessed. It is seen that even though the electricity generated by the BIGCC was greater than the CHPS by a factor of 2.6, the amount of steam generated was reduced by 22.6% when compared to CHPS. This in turn had restricted the amount of steam available to the integrated ethanol-sulphite process and thus, the restricted potential to displace the equivalent amount of coal corresponding to the steam supply. Thus, the overall displacement of coal resulting from the BIGCC technology was decreased by 25.5% when compared to the CHPS, because it was now limited by the lower amount displaced by steam.

The NGGRP of the scenarios that used bark to generate heat and power only (i.e. CHPS and BIGCC) was greater by 49.1%, on average, than the NGGRP of the scenarios that considered the combination of a gasification-synthesis process using the bark. This was expected since the exclusive generation of heat and power displaced coal while the BE-S combination scenarios improve the displacement of fossil hydrocarbon fuels, and the combustion reactions of coal and hydrocarbons shows that coal emits 0.03 kg of CO_2 per MJ while hydrocarbons emit 0.01 kg of CO_2 per MJ. In general, supplementing the recovery boiler with biogas generated by biodigestion had improved the NGGRP of all scenarios by an average rate 16%, due to the minor displacement of coal due to the improved output of the recovery boiler.

The results of the total capital investment (TIC) of the scenarios simulated, as well as the base line scenarios determined in Chapter 5 in shown in Figure 19. The indication of economic feasibility that was quantified by the average IRR (determined from Monte Carlo Economics) is

shown in Figure 20. Figure 20 also depicts the financial risks to a private investor, which was quantified as the probability of the IRR being less than 25% (Prob IRR <25%). Furthermore, the normalised NGGRPs of the scenarios are also depicted in this figure to illustrate the trade-off between economic viability and environmental benefits. Since Table 12 had shown that the utility generation from the methanol synthesis scenarios were not adequate to displace coal, and hence technically unviable, additional scenarios for methanol synthesis were considered for the economic analysis, where a portion of synthesis gas was diverted from the synthesis loop to the gas turbine, to provide enough utility output to satisfy the overall energy needs.

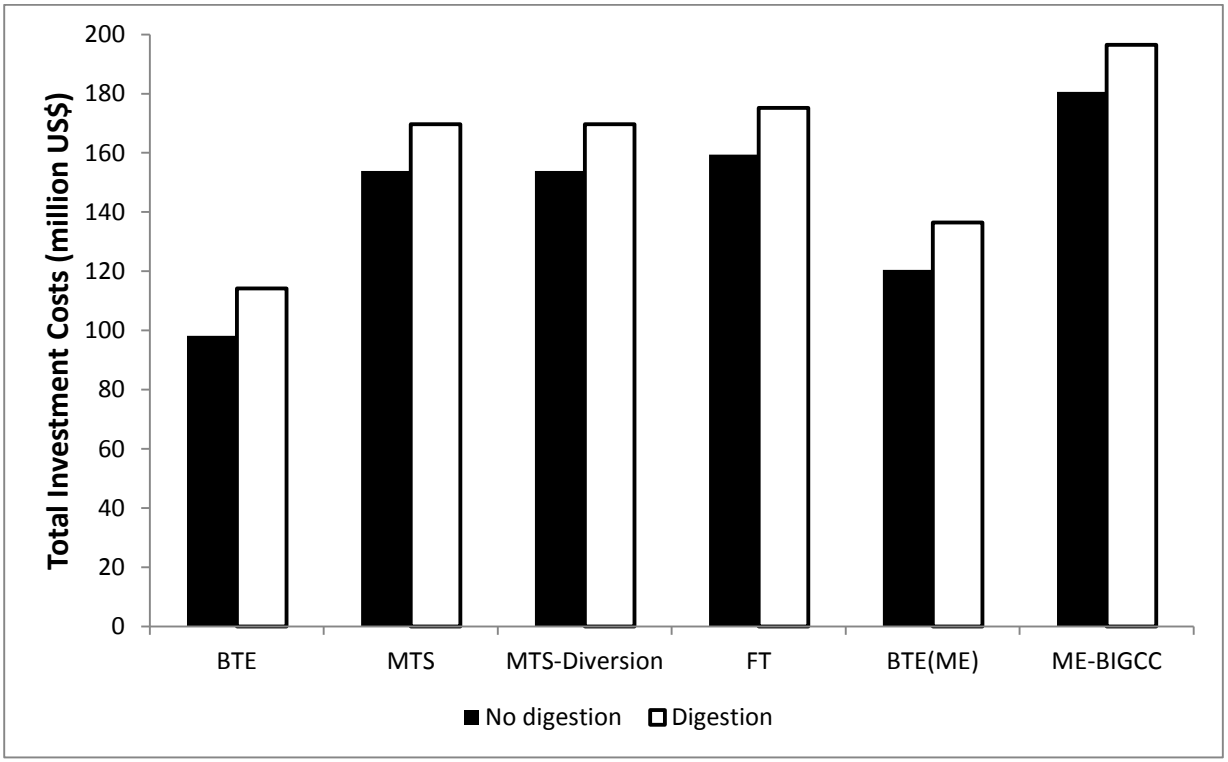


Figure 19: TIC of co-location scenarios (Conversion to heat and power via combustion BTE, and BIGCC; FTS – Fischer Tropsch Synthesis, MTS – methanol synthesis; ME – ethanol production with multi-effect distillation)

The highest TIC of 180.6 million US$ was attained for the 30-ME-BIGCC scenarios, which was approximately 50% higher than the relevant baseline scenario, which was the 30-ME-BTE. Thus, the effect of the higher capital and the lesser potential to displace the use of coal of this scenario (i.e.

30-ME-BIGCC) as shown in Table 12 at the integrated ethanol-sulphite facility resulted in an IRR that approached zero. Thus, the combination of BIGCC with ethanol generated from SSL does not have the synergetic effect with the multi-effect distillation as it was in Chapter 4 when a hemicellulose hydrolysate was fermented, due to the much lower concentration of ethanol in the beer product, which was at about 2%. Generally, feasible distillation of a fermentation beer would occur at an ethanol concentration of at least 4% [37]. Furthermore in chapter 4, the generation of electricity production had been maximised for sales and the excess generation of steam was minimised to prevent enthalpy from being wasted in the exhaust steam of the turbine[18], where as it is shown in Table 12 that the limited steam generation by BIGCC.

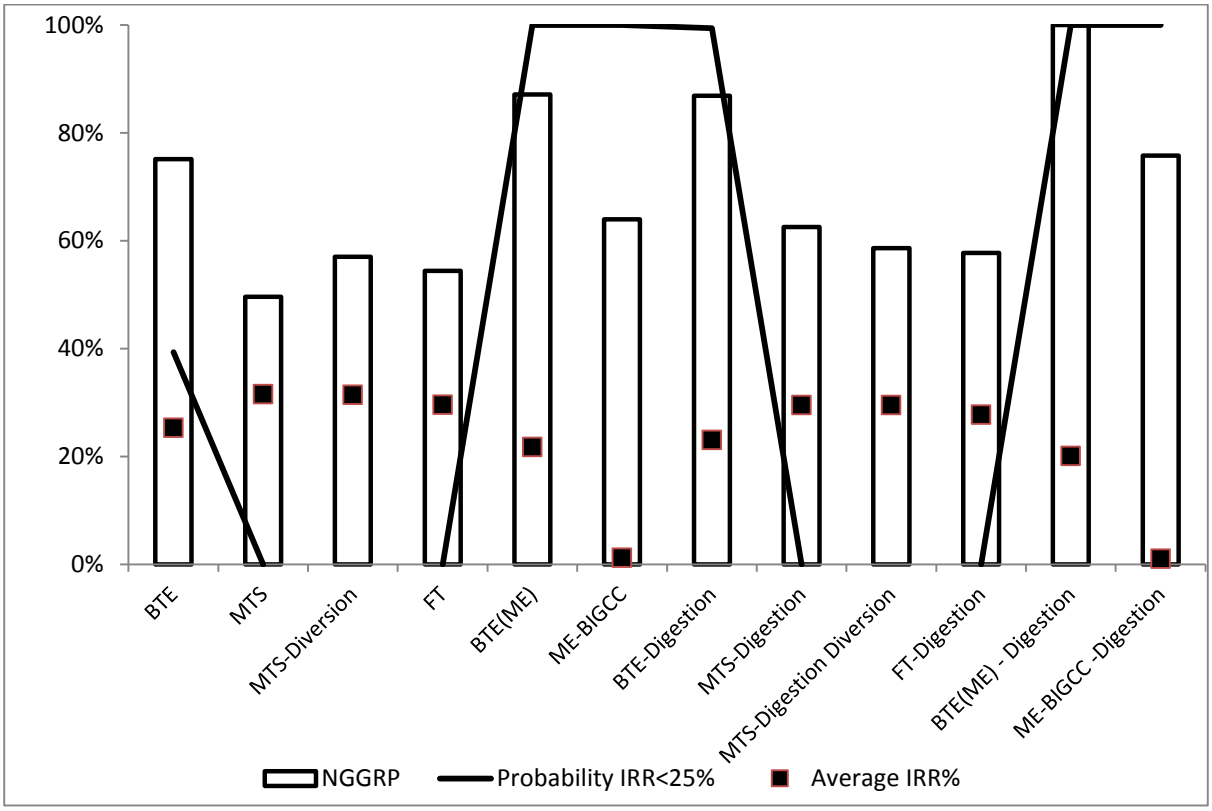


Figure 20: Economic Evaluation and trend in relative NGGRP (Conversion to heat and power via combustion BTE, and BIGCC; FTS – Fischer Tropsch Synthesis, MTS – methanol synthesis)

Relative to the 30-CON-BTE baseline scenarios, combining synthesis processes increased the TIC by 56.7 and 62.3% for methanol and FT synthesis, respectively. Even though the potential to displace coal had decreased, the respective increase in IRRs for FTS and MTS was 4.3 and 6.2%, resulting in a zero risk of lacking the returns expected by private investment. The negative costs associated with attaining feedstock (i.e. avoided disposal costs, conservatively estimated 8 $/ton, where literature estimates are about 13 $/ton[38]) was a primary contributing factor to the high economic feasibility, in contrast to a previous investigation, where FT synthesis from biomass was shown to have unfavourable returns in the South African context, because the feedstock price was 80U$ (2010) per dry ton[39]. It is also noted in these results that the difference in economic viability between MTS and FTS is marginal when compared to the difference in economic viability of these processes when integrated into a sugar mill, as shown in Chapter 6. This is due to the context of combining with ethanol production, where the differences in the overall investment costs between FTS and MTS scenarios are effectively decreased, due to the additional sharing of infrastructural costs, such as the Balance of Plant and Site Development costs, with the ethanol production process.

With regards to the trade-offs between environmental and economic benefits, Figure 20 shows that the opposing trends are generally maintained. While biodigestion improved the NGGRP, it also lowered the economic viability slightly, due to the increased capital. More importantly, it did not affect the zero-risk status of the co-location scenarios for private investment.

When syngas was diverted in the attempt to maintain the overall energy balance, it is seen that the IRRs are reduced by about 1%, due to the reduction in the methanol yield. In the case where biodigestion was used to supplement that energy supply, the methanol yield had reduced by 0.4% to maintain the energy balance; while in the absence of biodigestion, the yield of methanol reduced by 3.5% since the demand on the amount of syngas that was needed for diversion for utility production had increased. In terms of the greenhouse gas emissions, maintaining the energy balance through diverting syngas had improved the NGGRP by 15-18% on the scenarios without diversion, since coal was now displaced, rather than purchased.

5 Conclusions

In this chapter, various combinations of process technologies for the combination of synthesis fuel and ethanol production, integrated into a Sulphite mill were studied. Optimisation of the syngas production from bark had shown that atmospheric allothermal systems were advantageous compared to pressurised gasification, since its costs were less than half and with only an 18% decrease in efficiency. Considering the combination of synthetic and ethanol scenarios, Fischer Tropsch and methanol synthesis had Internal Rates of Return that was on average, 5.3% higher than the baseline ethanol production scenario where bark used to generate heat and power utilities. Subsequently, there were no risks imposed on private investment. Furthermore, it was shown that combining advanced ethanol purification techniques and power production using BIGCC had failed from an economic perspective. In terms of the net greenhouse gas reduction, the reduction potentials of the synthetic-ethanol combination scenarios were highly positive, even though it was 28% lower than the reduction potential of the base scenarios, on average. The utility supply from the methanol synthesis combination scenario was not adequate to maintain the overall energy balance, and therefore was modified to improve the utility production. These modifications had consequently reduced the methanol yield but did not however, have any significant impact on the economic potential on combining methanol synthesis and ethanol production from SSL.

6 Abbreviations

Abbreviation	Description
SSL	Spent Sulphite Liquor
CON	Conventional Distillation
ME	Multi-effect distillation
BIGCC	Biomass Integrated Gasification and

	Combined Cycles
AUT-G	autothermal gasification
ALO-G	allothermal gasification
AME	Amortised Capital Expenditure
CSP	Cost of Syngas Production
HRSG	Heat Recovery Steam Generator
AUT-G	autothermal gasification
OOC	operational opportunity cost
CE	Conversion Efficiency
MTS	Methanol Synthesis
FT	Fischer-Tropsch
IRR	Internal Rate of Return
NGGRP	Net Greenhouse Gas Reduction Potential

7 References

[1] Ekbom T, Lindblom M, Berglin N, Ahlvik P. Technical and Commercial Feasibility Methanol / DME Production as Motor Fuels for Automotive Uses - BLGMF. Brussels: 2003.

[2] Naqvi M, Yan J, Dahlquist E. Bioresource Technology Black liquor gasification integrated in pulp and paper mills : A critical review. Bioresour. Technol. 2010;101:8001–15.

[3] Consonni S, Katofsky RE, Larson ED. Chemical Engineering Research and Design A gasification-based biorefinery for the pulp and paper industry. Chem. Eng. Res. Des. 2009;7:1293–317.

[4] Huang H-jiang, Ramaswamy S, Al-dajani WW, Tschirner U. Process modeling and analysis of pulp mill-based integrated biorefinery with hemicellulose pre-extraction for ethanol production : A comparative study. Bioresour. Technol. 2010;101:624–31.

[5] Magdzinski L. Tembec Temiscaming Integrated Biorefinery. Pulp & Paper Canada 2006;107:147–9.

[6] Petersen AM, Haigh K, Görgens JF. Techno-economics of Integrating Bio-Ethanol Production from Spent Sulphite Liquor for Reduction of Greenhouse Gas Emissions from Sulphite Pulping Mills. Biotechnol. Biofuel. 2014;7:169.

[7] U.S. Environmental Protection Agency. Available and Emerging Technologies for Reducing Greenhouse Gas Emissions from the Pulp and Paper Manufacturing Industry. North Carolina: 2010.

[8] Hamaguchi M, Kautto J, Vakkilainen E. Chemical Engineering Research and Design Effects of hemicellulose extraction on the kraft pulp mill operation and energy use : Review and case study with lignin removal. Chem. Eng. Res. Des. 2013;91:1284–91.

[9] Landalv I, Furusjo E, Stare R. Patent WO2011123034A1 - Gasification of sulphite thick liquor - Google Patents. WO2011123034 A1, 2013.

[10] Tuna P, Hulteberg C, Hansson J, Asblad A, Andersson E. Synergies from combined pulp & paper and fuel production. Biomass Bioenerg. 2012;40:174–80.

[11] Holmgren KM, Berntsson T, Andersson E, Rydberg T. System aspects of biomass gasification with methanol synthesis e Process concepts and energy analysis. Energy 2012;45:817–28.

[12] Petersen AM, Farzad S, Görgens JF. Techno-economic assessment of integrating methanol or Fischer – Tropsch synthesis in a South African sugar mill. Bioresource Technology 2015;183:141–52.

[13] Helle SS, Murray A, Lam J, Cameron DR, Duff SJB. Xylose fermentation by genetically modified Saccharomyces cerevisiae 259ST in spent sulfite liquor. Bioresour. Technol. 2004;92:163–71.

[14] Helle SS, Lin T, Duff SJB. Optimization of spent sulfite liquor fermentation. Enzyme and Microbial Technology 2008;42:259–64.

[15] Laser M, College D. Comparative analysis of effi ciency , environmental impact , and process economics for mature biomass refi ning scenarios. Biofuels Bioproducts and Refining 2009;3:247–70.

[16] Ekbom T, Hjerpe C, Hermann F. Pilot study of Bio-jet A-1 fuel production for Stockholm-Arlanda Airport. Stockholm: 2009.

[17] Amigun B, Gorgens J, Knoetze H. Biomethanol production from gasification of non-woody plant in South Africa : Optimum scale and economic performance. Energ. Policy 2010;38:312–22.

[18] Petersen AM, Aneke M, Gorgens JF. Techno-economic comparison of ethanol and electricity coproduction schemes from sugarcane residues at existing sugar mills in Southern Africa. Biotechnol. Biofuel. 2014;7:1–19.

[19] ANDRITZ Group. ANDRITZ Recovery Boilers n.d.

[20] Moor B. MODERN SUGAR EQUIPMENT ASSISTING COGENERATION. 2008.

[21] Rodrigues M, Walter A, Faaij AP. Performance evaluation of atmospheric biomass integrated gasifier combined cycle systems under different strategies for the use of low calorific gases. Energy Conversion and Management 2007;48:1289–301.

[22] Craig KR, Mann MK. Cost and Performance Analysis of Biomass-Based Integrated Gasification Combined-Cycle (BIGCC) Power Systems Cost and Performance Analysis of Biomass-Based Integrated Gasification Combined-Cycle (BIGCC) Power Systems. National Renewable Energy Laboratory 1996.

[23] Jantsch TG, Angelidaki I, Schmidt JE, Brana de Hvidsten B., Ahring BK. Anaerobic biodegradation of spent sulphite liquor in a UASB reactor. Bioresour. Technol. 2002;84:15–20.

[24] Liu G, Larson ED, Williams RH, Kreutz TG, Guo X. Making Fischer-Tropsch Fuels and Electricity from Coal and Biomass: Performance and Cost Analysis. Energy and Fuels 2011;25:415–37.

[25] Niederl A, Narodoslawsky M. Life Cycle Assessment – study of Biodiesel from Tallow and Used Vegetable Oil. Institute for Resource Efficient and Sustainable Systems 2004.

[26] Wiloso EI, Heijungs R, Snoo GRD. LCA of second generation bioethanol : A review and some issues to be resolved for good LCA practice. Renew. Sustain. Energ. Rev. 2012;16:5295–308.

[27] Sheehan J, Aden A, Paustian K, Killian K, Brenner J, Walsh M, et al. Energy and Environmental Aspects of Using Corn Stover for Fuel Ethanol. Journal of Industrial Ecology 2004;7:117–46.

[28] Petersen A, Melamu R, Görgens J., Knoetze, J.HCheng H. Comparison of Second-Generation Processes for the Conversion of Sugarcane Bagasse to Liquid Biofuels- Part A: Energy efficiency, Pinch Point Analysis and Life Cycle Analysis. Energy Conversion and Management 2015;91:292–301.

[29] Rebitzer G, Ekvall T, Frischknecht R, Hunkeler D, Norris G, Rydberg T. Life cycle assessment Part 1 : Framework , goal and scope definition , inventory analysis , and applications. Environment International 2004;30:701–20.

[30] Palou-rivera I, Wang M. Updated Estimation of Energy Efficiencies of U.S. Petroleum Refineries. Center for Transportation Research Argonne National Laboratory 2010:1–6.

[31] Wang M, Burnham A, Wu Y. GREET 2007.

[32] Elsayed MA, Matthews R, Mortimer ND. CARBON AND ENERGY BALANCES FOR A RANGE OF BIOFUELS OPTIONS. 2003.

[33] Richardson JW, Herbst BK, Outlaw JL, Anderson DP, Klose SL, Gill II RC. Risk Assessment in Economic Feasibility Analysis: The Case of Ethanol Production in Texas. 2006.

[34] Richardson JW, Lemmer WJ, Outlaw JL. Bio-ethanol Production from Wheat in the Winter Rainfall Region of South Africa : A Quantitative Risk Analysis. Int. Food. Argibus. Manag. Rev. 2007;10:181–204.

[35] Amigun B, Petrie D, Görgens J. Economic risk assessment of advanced process technologies for bioethanol production in South Africa : Monte Carlo analysis. Renewable Energy 2011;36:3178–86.

[36] Channiwala S, Parikh P. A unified correlation for estimating HHV of solid, liquid and gaseous fuels. Fuel 2002;81:1051–63.

[37] Ohgren K, Rudolf A, Galbe M, Zacchi G. Fuel ethanol production from steam-pretreated corn stover using SSF at higher dry matter content. Biomass Bioenerg. 2006;30:863–9.

[38] Johannessen LM, Boyer G. Observations of Solid Waste Landfills in Developing Countries: Africa, Asia and Latin America. Washington D.C.: 1999.

[39] Leibbrandt NH. Techno-Economics Study for Sugarcane Bagasse to Liquid Biofuels in South Africa: A Comparison between Biological and Thermochemical Process Routes. PhD Dissertation Department of Process Engineering. University of Stellenbosch, University of Stellenbosch 2010.

Chapter 8: Conclusions and Recommendations

In this dissertation, detailed process flow sheet analyses were conducted to arrive at feasible processing options, for integrating biofuel production from residues generated at the Sugar Cane Crushing (SCCI) and Paper and Pulp industries (P&PI) in South Africa. In South Africa, the SCCI is represented by the Raw Sugar Industry (RSI) (i.e. the sugar mills) and the residues generated are sugarcane bagasse and trash, while the Sulphite Pulping Process with Spent Sulphite Liquor (SSL) and bark generated as residues represented the P&PI. A feasible integrated scenario entailed that the energy needs of the host facility was not compromised in a significant manner, and that the scenario provided the attractive returns for a private investment, based on acceptable product yields, while maintaining a greenhouse gas reduction throughout the biofuel lifecycle. Furthermore, yields of energy products for export were maximised through the application of energy efficiency optimisation (e.g. pinch analysis) to integrated process scenarios. The main conclusions from these objectives are discussed in this chapter.

1 Conclusions on the various options of integrating biofuels into the RSI and P&PI of South Africa

The detailed conclusions of all the scenarios evaluated in this dissertation are represented in Table 13, which summarises the performances on facilities with integrated biofuels production, in terms of the (bio-)energy self-sufficiency, economic viability and greenhouse gas reduction (GHG) potential, where applicable. For the various approaches to biofuel integration considered, Table 13 is presented in four parts, and detailed discussions follow:

A. Integration of bioethanol production into the RSI

B. Integration of synthetic fuel production into the RSI

C. Integration of bioethanol production into the P&PI

D. Integration of combined synthetic fuel and bioethanol production in the P&PI

Table 13: Detailed Conclusions of Integration Scenarios Studied

Scenarios	Energy Self-sufficient?	Economic Viability?	GHG reductions	Recommended for implementation
PART A: Integration of bioethanol production into the RSI				
Legend: Prob(IRR)<25%, probability that IRR recedes below 25%; CPE, coproduction of ethanol and electricity; EE, electricity exclusive generation; CON, conventional distillation; VAC, vacuum distillation, CHPSC, combustion with high pressure steam cycles; BIGCC, biomass integrated gasification with combined cycles; Export efficiency = (Export Electricity + Higher Heating Value of Ethanol Produced)/(Higher Heating Value of Biomass Residues)				
CPE-CON-BIGCC	Yes (with export efficiencies ranging from 25-33% for CPE and 15-27% for EE)	Yes, Prob(IRR)<25%=7%	Yes	No. Steam production not adequate.
CPE-VAC-BIGCC		Yes, Prob(IRR)<25%=0%		Yes
CPE-CON-CHPSC		Yes, Prob(IRR)<25%=0%		Yes
CPE-VAC-CHPSC		Yes, Prob(IRR)<25%=1%		No. Lower efficiency than other options.
CHPSC - EE		No, Prob(IRR)<25%=80%		No.
BIGCC - EE		Yes, Prob(IRR)<25%=2%		Yes
PART B: Integration of synthetic fuel production into the RSI				
Legend: MTOH, methanol synthesis; FT, Fischer-Tropsch crude synthesis; CVN, conventional reactor configuration; AD, advanced reactor configuration; IE, imports electricity to fulfil the energy balance; ING, imports natural gas to fulfil the energy balance; DIV, diversion of syngas to fulfil the energy balance				
MTOH-CVN	No	No, Prob(IRR)<25%=100%	Yes	No. Economically unfeasible, and not energy self sufficient
MTOH-AD	No	No, Prob(IRR)<25%=97%		No. Economically unfeasible, and not energy self sufficient
FT-CVN	Yes	No, Prob(IRR)<25%=100%		No. Economically unfeasible.
FT-AD	Yes	No, Prob(IRR)<25%=100%		No. Economically unfeasible.
MTOH-CVN-IE	No	No, Prob(IRR)<25%=100%		No. Economically unfeasible, and not energy self sufficient
MTOH-AD-ING	No	No, Prob(IRR)<25%=100%		No. Economically unfeasible, and not energy self sufficient
MTOH-AD-DIV	Yes	No, Prob(IRR)<25%=100%		No. Economically unfeasible.
PART C: Integration of bioethanol production into the P&PI				
Legend: MESP, minimum ethanol selling price; ISP, international selling price; mean(IRR), arithmetic average of IRR from Monte Carlo simulation; 20DS, feed SSL with dissolved solids at 20%; 30DS, feed SSL with dissolved solids at 30%; ME, multi-effect distillation; CON, conventional distillation; CS, coal supplementation; BB, boiler fuelled with bark; BD, biogas supplementation from effluent digestion; TAC, SSL feed with time averaged characteristics				
20DS-ME-CS	n/a; base-line scenarios	No, mean(IRR)<25%	GHG accrual due to coal	No. Not economic viability for private investment
20DS-CON-CS				
30DS-ME-CS				
30DS-CON-CS				
20DS-ME-CS-BD	No; energy supplementation by	No, mean(IRR)<25%		
20DS-CON-CS-BD				

30DS-ME-CS-BD 30DS-CON-CS-BD	biodigestion supplementation insufficient			
20DS-ME-BB 20DS-CON-BB 30DS-ME-BB 30DS-CON-BB	Yes; and reduces the overall reliance of the mill on coal for energy demands	No, mean(IRR)<25%	GHG reductions in addition to reducing carbon footprint of host industry	
20DS-ME-BB-BD 20DS-CON-BB-BD 30DS-ME-BB-BD		No, mean(IRR)<25%		
30DS-CON-BB-BD		no, Prob(IRR)<25%=20%; but MESP>ISP		
30DS-CON-BB-BD-TAC		Yes, Prob(IRR)<25%=20%; & MESP<ISP		Yes. GHG reductions and low risk for private investment
Part D: Integration of combined synthetic fuel and bioethanol production in the P&PI				
Legend: 30DS, feed SSL with dissolved solids at 30%, FT, Fischer-Tropsch crude synthesis; MTOH, methanol synthesis; CON, conventional distillation of ethanol; VAC, vacuum distillation of ethanol; DIV, syngas diversion to fulfil the energy balance; BD, biodigestion of effluent				
30DS-VAC-BIGCC	Yes	No, Prob(IRR)<25=100%	Yes.	No. Economically unfeasible
30DS-CON-MTOH	No	Yes, Prob(IRR)<25=0%		No. Economically feasible, BUT not energy self sufficient
30DS-CON-FT	Yes	Yes, Prob(IRR)<25=0%		Yes. Economically feasible, energy self-sufficient
30DS-CON-MTOH-DIV	Yes	Yes, Prob(IRR)<25=0%		Yes. Economically feasible, energy self-sufficient.
30DS-VAC-BIGCC-BD	Yes	Yes, Prob(IRR)<25=0%		No. Economically unfeasible
30DS-CON-MTOH-BD	No	Yes, Prob(IRR)<25=0%		No. Economically feasible, BUT not energy self sufficient
30DS-CON-FT-BD	Yes	Yes, Prob(IRR)<25=0%		Yes. Economically feasible, energy self-sufficient
30DS-CON-MTOH-DIV-BD	Yes	Yes, Prob(IRR)<25=0%		Yes. Economically feasible, energy self-sufficient

1.1 Integration of Second Generation Biofuels Production in the Raw Sugar Industry

1. Concerning the integration of bioethanol co-production process routes (Table 13 Part A):

- A process configuration based on hemicellulose extraction for ethanol fermentation, followed by conventional ethanol purification through atmospheric distillation, and the conversion of cellulose and lignin residue from hemicellulose extraction to heat and power, through high pressure boilers had an overall efficiency and IRR of 26% and 28%, respectively (i.e. CPE-CD-CHPSC), and was thus recommended for future investment. This Internal Rate of Return was obtained under conservative estimates of the selling prices of the export

products, and there was no significant risk to private investment, since the probability of the IRR falling below 25% was less than 20%. A major difference between this scenario and those typically considered for ethanol integration in literature was that enzyme costs was not part of the production costs, which gave this scenario better investment potential. Thus, it can be concluded that enzyme cost is still a major economic hindrance to the conversion of cellulose to ethanol, and that avoiding this cost through ethanol production from hemicellulose alone, would provide viable investment opportunities in second generation bio-ethanol production.

- Employing advanced technologies such as multi-effect distillation and Biomass Integrated Gasification and Combined Cycles (BIGCC) in combination with ethanol production from hemicellulose (i.e. CPE-VD-BIGCC) had an overall net efficiency of 32% and an IRR of 29% and was attractive to private investors due to low financial risk. The increase in efficiency was attributed to the greater efficiency of the BIGCC technology in generating electricity from the pre-treatment residue. Thus, there will be even more promising options for ethanol co-production with electricity export at sugar mills in future with the maturation of advanced electricity generation technologies. For such technologies however, it is recommended that the efficiencies of sugar mills are improved from 0.4 tons of steam per ton of cane to below 0.35 tons, which had been shown as a foreseeable target is the future. This is recommended because the BIGCC technology was incapable of satisfying the combined steam demand of ethanol production and sugar-mill.
- Since the maximum IRR, in terms of the weighted-average capital cost, allowed for Independent Power Producers under South African legislation is 17%, it makes bioethanol production a more feasible use of sugarcane residues than the exclusive production of electricity. Without this restriction however, BIGCC-EE will obtain IRRs that are similar to bioethanol scenarios. While exclusive electricity only benefits the electricity supply, co-production benefits the energy sector by also reducing the reliance of the transportation

fuel demand on fossil sources, which in itself is a major source of greenhouse gas reductions in South Africa.

2. Concerning the integration of synthetic fuel production routes into existing sugar mills (Table 13 Part D)

- The most cost effective configuration for producing clean compressed syngas from sugarcane residues was allothermal gasification. Though this method was 25% less efficient than autothermal systems, the overall syngas cost was 61% less. This process avoided the costs associated with oxygen production. Furthermore, the integrated process was energy self-sufficient, due to the steam and potential electrical energy generated by the combustion chamber. Thus, as the major costs in gasification-synthesis processes occur in the production of clean, compressed syngas, using allothermal technologies for gasification of biomass residues with optimised parameters is an essential step to reducing the overall costs of synthetic fuel production.
- Conventional synthesis technologies (FT-CON and MTOH-CON) that entail gas phase reactors and recycle loops for Fischer-Tropsch (FT) and methanol synthesis had efficiencies ranging from 25 to 33%, but with poor economic feasibilities, since the IRRs ranged at 8-16%, and definitely failing to provide returns on private investment. Advanced technologies (FT-AD and MTOH-AD) for FT and methanol synthesis had better technical and economic performances, since the efficiencies range at 33-38% and IRRs range from 17-21%. There is still however, no incentive for private investment since the risk of the IRRs receding below 25% was too high, especially with the FT syncrude option since the value of the syncrude product itself is too low. Furthermore, a methanol synthesis process was shown to require an additional energy source to fulfil the thermal-energy requirements of the hosting sugar mill, implying that an integrated methanol synthesis process would not have a self-sufficient energy balance even with the maximum use of the available residues. Therefore, integration

strategies at sugar mills that considers gasification-synthesis pathways are not options that can be considered in the mid-term. These routes should be reassessed in future when the advanced methanol reactor technologies has matured and when the sugar mills themselves are more efficient, so that the production of methanol from the residues does not compromise the energy needs.

3. Comparison between synthetic fuel and biological processing routes for integration.

- The highest net exporting efficiency attained by the synthesis routes is 38% while that attained by biological routes is 32%. The synthesis routes however, had in some instances required an import of fossil energy at a rate ranging at 1-4% of the total calorific input in order to fulfil the steam demand of the mill. Regarding the bioethanol route, a supplementary source of energy was not required, but the process made use of reagents and chemicals for the fermenting micro-organisms to grow and function. Thus, both technologies introduce minimal greenhouse gas emissions into the life cycles of the fuels, and thus, efficiency and environmental benefits would not provide a basis to differentiate these biofuel processes.
- Bioethanol processes have greater economic feasibility than synthetic fuels, as IRRs in excess of 29% could be attained, with no significant risk to private investors, whereas the IRRs for the synthetic routes were below 22%. Therefore, bioethanol routes scenarios are available for the mid-term, while bioethanol production with advanced technologies would compete with gasification-synthesis processes as technology for the latter matures.

1.2 Integration of Second Generation Biofuels Production into the Sulphite Pulping Process

1. With regards to production of bioethanol at Sulphite processes (Table 13 Part C).

- Fermentation of SSL should be done at solids concentrations of approximately 30% (30DS), as the higher yields obtained by fermentation in more dilute conditions (20DS) were negated by very high energy costs in downstream ethanol recovery. These downstream energy and process costs mostly occurred in the distillation section, and these costs were accentuated when multi-effect distillation (VAC) was considered. Thus, when a process that produced a low-value product like ethanol was considered where the process feed streams were in an excessively diluted state, the yield of the product was traded-off with the efficiencies in process energy management.
- If coal was used to supply the net energy demand needed for ethanol production (see CS scenarios), then a net increase in life cycle greenhouse gas emissions occurred, rather than the desired reduction in GHG emission. This would render ethanol from such a process as a non-sustainable product, from a global warming perspective. This phenomenon can be attributed to the dilute conditions at which ethanol is produced by fermentation of SSL, when compared to the use of coal for process energy in corn-ethanol production. The fermentation broth in the latter case had contained 70 to 110g/l ethanol (see Literature Review, Chapter 2), thus requiring lower distillation energy inputs than SSL fermentations, allowing (marginal) greenhouse gas reductions to be obtained in the life cycle of the fuel.
- Maximising the use of the renewable energy available in the other biomass residues (see BB and BD scenarios) instead of supplementation of process energy supply with coal, was achieved by converting the bark to heat and power through combustion, and by anaerobic digestion of the discharge liquid effluents to supply biogas as energy. As a result, the integrated pulping-ethanol processes achieved a net reduction in greenhouse gas emissions, by displacing a portion of the coal needed to power the sulphite process with excess heat and power from bio-energy sources. Thus, it is essential that the process energy requirements of an ethanol process, especially with dilute feedstocks and products, are

provided by renewable energy sources, to maintain a net greenhouse gas reduction in the life cycle of the fuel.

- The economic risks imposed on private investors by the process scenario with net reduction greenhouse gas emissions were significant when the process feedstock characteristics where based on an SSL sample that was relatively dilute. Using a process feedstock based on SSL that had more concentrated characteristics, reflective of a time averaged composition of the stream (see 30DS-CON-BB-BD-TAC scenario), the risks were reduced considerably, making the integrated ethanol process economically feasible. Therefore, since flow sheet analysis has shown that industrial application of recombinant xylose fermenting yeasts to a pentose dominated SSL substrate is economically feasible, another integrated biofuel process for the P&PI is possible in addition to those already explored in literature.

2. Regarding the combination of synthetic fuel and bioethanol fuels for integration into the sulphite pulping process (Table 13 Part D)

- The bark should be converted to syngas using allothermal gasification, because the overall costs were low when compared to pressurised autothermal gasification. This result is in accordance with what was determined for the gasification of residue in the raw sugar industry (Table 1, Part D). However, the difference in the cost in the SCCI between allothermal and autothermal techniques was 80% while the difference in the P&PI was 64%. Considering that the heating value of bark is 28% higher than sugarcane residues, this comparison suggests that the selection of gasification technology for biomass is dependent on the calorific value of the biomass.
- Combining synthesis fuel production from bark at an integrated ethanol-sulphite process (30DS-CON-FT, 30DS-CON-MTOH) offers high economic return with IRRs that had ranged from 28 to 32%, with no risk to private investment. This was attributed to the negative cost of the bark as feedstock to the synthetic process and because the low value utilities

generated by the synthetic fuel process powered the generation of a high value product like ethanol, instead of only displacing a low value product like coal. Compared to scenarios where only ethanol was produced and bark used for heat and power generation (30DS-CON-BB; 30DS-VAC-BIGCC), co-locating thermochemical process improved the liquid yield by up to a factor of 5, while the net reductions in GHG emissions achieved by the combined process, decreased by about 50%. Therefore, provided that the exothermic energy released by the gasification-synthesis process sustains the bioethanol energy needs, the economic feasibility of biofuel production can be enhanced by considering combined synthesis fuel and bioethanol production, as overall fuel yields are enhanced. Thus, better economic performances are achieved by combining synthetic fuel with bioethanol production, even though it comes at the expense of GHG reduction emissions.

-

2 Summary of Conclusions in relation to the Overall Research Question

This dissertation had shown that through detailed simulation and assessment of the technical, economic and greenhouse gas reduction potential of processing options, certain strategies for the integration of biofuel production into the existing biomass processing industries can serve as attractive opportunities for private investment in South Africa, specifically by utilisation appropriate forms and quantities of residues from these biomass processing facilities. For the RSI, the current opportunity lies in the bioethanol production coupled with electricity generation systems that are combustion-based (CPE-CON-CHPSC). If the steam demands of sugar mills reduce below 0.4 tons per tons of cane, then future implementation could consider ethanol production with BIGCC-based energy generation systems (CPE-VAC-BIGCC), or methanol production via thermochemical conversion (MTOH-AD), once these technologies are successfully demonstrated and are available at matured costs.

In terms of the P&PI, an economically viable process may lie in the production of bioethanol from a pentose rich digestion liquor at Sulphite processes, provided that the pulp digestion process itself operates optimally, so that the concentration of sugars in the SSL is at least 25g/l when it leaves the digestion reactors (30DS-CON-BB-BD-TAC). For further consideration of this process, optimising the impact caused by the resulting chemical modifications that bioethanol production imposes on the chemical characteristics of the SSL, which in-turn affects the chemical recovery process, must be evaluated. Therefore, the current interests of private investors in South Africa for second generation biofuels should firstly focus on the prospective process in the RSI that is based on technology that is currently demonstrated.

The ultimate potential for integration in this study was demonstrated by bio-refinery concepts that considered the combination of bioethanol and gasification-synthesis scenarios at Sulphite mills (30DS-CON-FT, 30DS-CON-MTOH-DIV). Such concepts were shown to be highly lucrative from a financial perspective, even at small scales, with the restraints that at least some of the residues are obtained at avoided costs. Otherwise, such concepts are expected to be most profitable because they take full advantage of the sharing of infrastructure and Balance of Plant (BOP) costs between the sub-processes of the bio-refinery. Furthermore, combining these processes ensure that only higher value products are exported as waste heats from the synthesis processes are used to supply energy for ethanol production. Thus, while gasification-synthesis processes as combination scenarios integrating in the P&PI are lucrative, they were not lucrative when integrating in the RSI because the integrated methanol scenario was not self-sufficient and because the FT synthesis process produced large amounts of waste heat. Furthermore, the capital costs specific to the gasification synthesis processes were high, as the BOP costs are not shared with a combined facility.

While the contexts of combining processes in the P&PI had promoted synthesis processes when compared to the RSI, it had the opposing effect on Heat and Power generation schemes. This occurred because heat and power generation in the RSI resulted in the sale of an electricity product that had a value at 0.03US$/MJ (2012) (which was similar to the fuel prices), while heat and power production combined with ethanol production in the P&PI had only resulted in the displacement of coal, which only carried a value of 0.005US$/MJ (2012). Thus, the technical and financial contexts that an industry offers is found to ultimately dictate which process technology would be most suited.

In this dissertation it was shown that integrated biofuel production scenarios with high economic returns that were reflected by IRRs in excess of 25% are possible. Such numbers had exceeded the IRR determinations in literature, due to circumstances and technological options that were not explored in integration concepts. It already been noted in this Conclusions Chapter and Chapter 4 that a process that exploited the negation of enzyme costs had greatly reduced the costs of ethanol production integrated into the sugarcane crushing industry. Furthermore, a premium price afforded on the electricity generated from renewable sources in South Africa had further improved the IRRs attained in this dissertation. In the context of Sulphite mills, the ethanol production costs were reduced because of the negation of enzyme costs, in addition to the negation of the costs of hemicellulose solubilisation, which was provided by Pulp Digestion in the Sulphite Process. The IRR achieved for integrated gasification-synthesis scenarios (in the RSI) did not show any significant increase to that determined in literature, as the overall synthetic processes and product prices were similar.

3 Novelty of Work

In this study, flow sheet analyses were used to determine interactions of alternative technologies in a processing stage with downstream technologies and the respective limitations in detailed process integration studies of biofuels with industries. In ethanol co-production with electricity export, multi-effect distillation was found to be synergetic with BIGCC energy generation while conventional distillation was synergetic with combustion based processes. Multi-effect distillation however, was shown to be inapplicable when feed substrates are limited to low sugar concentrations, such as SSL. With further reference to SSL, it was shown through flow sheet analysis that the substrate concentrated to 20% solids is undesirable even though it promoted higher microbial conversion than the 30% solid concentrations, due to the higher energy demand that such conditions caused downstream. Furthermore, it was generally shown for ethanol processes based on substrates that were limited to low sugar concentrations, that it is essential for the energy demands to be sourced from renewable sources so that the life cycle of the biofuel does not accrue greenhouse gas emissions.

A method of flow sheet analyses that coupled process simulation outcomes and economic analysis with statistical evaluations was used to optimise and compare competing technologies for a processing stage in particular contexts. Specifically, competing technologies for syngas generation was optimised for selection in a synthesis flow sheet that is to be integrated into the SCCI and P&PI with the rationale that the major costs of gasification-synthesis processes lies in syngas production and preparation. In these particular contexts, optimised syngas production technologies based on allothermal gasification was more suitable. Thus, a novel approach in optimising the technical and economic aspects producing of clean, compressed syngas was carried out as an essential step in

developing a feasible synthetic fuel production process from biomass when integrated into host industries, which are in themselves energy intensive.

Through flow sheet analysis of gasification-synthesis scenarios, it was also shown that integrating processes with high liquid fuel efficiency such as methanol synthesis are not technically viable for integration into the RSI that have steam demands at 0.4 tons per ton of cane, even when the waste heats generated by the synthesis process is used to generate low pressure steam for the sugar mill. Integrating a more exothermic process such as FT synthesis may be technically viable, but not financially viable due to the low liquid product yield and the low economic value of the liquid product. Thus, it was shown that the high capital costs associated with gasification-synthesis process was a hindrance for these processes to yield attractive investment opportunities to private investors, when integrated into the RSI.

Flow sheet analysis which considered the novel integration of combined synthetic fuel with bioethanol production at Sulphite pulping processes, which used all available residues generated, had shown promising results. Essentially, the primary beneficial factors of combined synthetic-bioethanol fuel production were the maximum yield of valuable products and the lowest overall capital costs per yield of product. In addition to the high yield of liquid, it was shown that the fossil fuels that are used to satisfy the energy balance of the mill are partly displaced. Furthermore, the use of a waste product like bark for synthetic fuel production negated the usual disposal costs and this contributed to a feasible implementation at a relatively small scale, if compared to the larger scale of its implementation in the RSI where it was economically unattractive, when costs were attached to the feedstock residues.

Lastly, it was seen that the overall performance and selection of competing technologies is ultimately dictated by the technical and financial contexts that the integration in a particular industry offers. In this study, integrating in the RSI was found to promote heat and power generation while integration combined scenarios in the P&PI was found to promote gasification-synthesis scenarios.

4 Recommendations for further research

The realisation of the full potential of the concepts proposed in this dissertation will come after the following questions and points that were not within the scope of this dissertation are researched or demonstrated thoroughly:

1. Micro-organisms that can efficiently ferment hemicellulose sugars in pre-treatment hydrolysates and SSL without the need for detoxification, in order to save on capital and chemical costs.
2. The effect of added dissolved salts in SSL due to detoxification on the operation of the recovery boiler system. As technical data on the operation of this system in not available in the public domain, it could not be simulated in this study. Thus, an approximate study could be employed to examine possible effects on ash formation and acid gas recovery, and subsequently, detoxification could be optimised for minimising the effect.
3. Catalytic gasification of biomass species that was able to produce tar free syngas should be demonstrated at an industrial level.
4. Details around the energy requirements of the host industries should be carried out in order to identify areas where low quality heat would suffice. This will then reduce the reliance on the live steam requirements, and will maximise the potential to integrate biofuel processes where low quality, reject heat is generated.

5. Explore and develop new factored heuristics for the estimates for the cost of Balance of Plant (BOP) and infrastructure that is required in the determination of the Total Investment Costs (TIC) for integrated biofuel processes at host industries. In this study, these costs were estimated based on heuristics for stand-alone facilities where BOP and infrastructure are developed from green-fields. In integrated biofuel production however, the existing BOP and infrastructure is only modified to accommodate the biofuel process. Therefore, heuristics based on this phenomenon rather than an estimate based on a green-field development will reflect the true potential of the reduction in the determination of TIC for integrated biofuel processes.

*******The End*******

APPENDICES

APPENDIX A: UNIT OPERATION SPECIFICATIONS

In this appendix, the specifications for the various unit operations is shown in the tables that follow, where units are categorised into the cases of their general applicability, such as bioethanol and synthetic fuel production units. The units categorised in energy generation (Table A 2) applies to both bioethanol (Table A 1) and synthetic fuel production (Table A 3), with some differences. Furthermore, cooling utility equipment is shown in Table A 4. In each table, the unit is described and areas of their applicability are given in reference to the chapters. Applicable reactions are also listed, and the unit specifications that were given as inputs into Aspen Plus are detailed.

Table A 1: Unit Operations in Bioethanol Production

Unit Operations	Applicability and description	Reactions	Conditions	Reference / Note
Pre-Treatment Reactor	Hemicellulose Extraction in Chapter 4, for sugarcane residues.	Cellulose + H2O --> glucose Cellulose + H2O --> cellubiose Xylan + H2O --> xylose Xylan + H2O --> Xylo-oligose Cellulose -> HMF Xylan --> Furfural + 2H2O 2Xylan + 2H2O --> 5Acetic Acid	Temperature = 210°C Pressure = 19.5bar	[1,2] [3]
Autothermal Hydrolysis	Conversion of oligomers to monomers in hemicellulose hydrolysate in Chapter 4.	Cellubiose+H2O->glucose Xylo-oligose+H2O ->xylose	Temperature = 120°C Agent: Acid added at 0.5%	[4]

			Residence Time = 20mins	
6-Effect Evaporator Concentration	Thermally concentrates the SSL from an initial dissolved solids concentration from 10% to 60%		Evaporator Pressures 0.1 atm 0.3 atm 0.5 atm 0.9 atm 1.3 atm 2.3 atm	a
Detoxification	Deactivation of inhibiting compounds in hemicellulose hydrolysate in chapter 4 and spent sulphite liquor in chapter 5	unspecified	Temperature = 30°C pH = 9 Residence Time = 1hr Agents: Ammonium hydroxide (sugarcane residue hemicellulose hydrolysates, Chapter 4) Sodium Hydroxide (SSL, chapter 5)	[5,6]

Seed Train/Cell Cultivation	Cells grown from purchased sugars and conditioned with sugarcane residue hemicellulose hydrolysate in Chapter 4 and SSL in Chapter 5	glucose --> 7.75*biomass xylose --> 6.47*biomass glucose + 6O2 --> 6CO2 + 6H2O Xylose + 5O2 --> 5CO2 + 5H2O	Temperature = 30°C Residence Time = 48hours, Fed-Batch mode	[7]
Fermentation	Fermentation of sugars in sugarcane hemicellulose hydrolysate in Chapter 4 and SSL in Chapter 5	hexose --> 2ethanol+2 CO2 3 pentose -->5ethanol+5CO2 glucose --> 7.75*biomass xylose --> 6.47*biomass xylose + H2O --> xylitol + 0.5 O2	Residence Time = 140 hours Temperature = 30°C	[8–11]
Crude Distillation Conventional/atmospheric	Recovery of ethanol from unconverted sugars at >99% recovery in sugarcane residue hemicellulose hydrolysate in Chapter 4,and unconverted sugars and		Trays = 13 Conventional/atmospheric pressure ~ 1.5atm Vacuum/multi-effect pressure = 0.2atm	[3,12]

	lignosulphonates in SSL in Chapter 5.			
Rectification Column	Recovery of ethanol from water and >99% recovery, with ethanol distillate at a mass concentration of about 92.5%.		Pressure = ~1.5 atm Trays = 18	
Molecular Sieves -	Purification of ethanol to a grade of 99.5%		Temperature = 120°C	[3]

a. Pressures estimated from temperatures given in Perin-Levasseur et al. [13] and plant data from Sappi Saiccor.

Table A 2: Energy Generation Equipment

Unit Operations	Applicability and description	Reactions	Conditions	Reference / Note
Combustion boiler	Combustion of sugarcane residues, raw and pre-treated (Chapter 4).	CHaOb + ((2-b)/2+a/4))O2--> CO2+(a/2)*H2O	Excess air --> for oxygen in flue gas to be >6%. Energy recovery from flue gas is reflective of	[14,15] a

	Combustion of concentrated SSL at 60% solids, and bark biomass and coal (Chapter 5+7).		a stack gas temperature of 130°C. Boiler Steam Pressure --> 80bar (from sugarcane biomass; Chapter 4 bark biomass Chapter 5+7) Boiler Steam Pressure --> 49bar, (from concentrated SSL and coal, Chapter 5+7)	b
Atmospheric air gasification for Biomass Integrated Gasification and Combined Cycles and Tar Cracking	Gasification of sugarcane residues, raw and pre-treated with air (Chapter 4). Gasification of bark biomass with air (Chapter 7).	$CHaOb + (1-b)H2O \rightarrow CO+(1-b-(a/2)H2$ $CHaOb + CO2 \rightarrow bH2O+2CO+((a/2)-b)H2$ $CHaOb + ((1-b)/2+a/4))O2 \rightarrow CO+(a/2)*H2O$	Biomass moisture = 15% Equivalence ratio of air set for temperature of 920°C for Tar cracking.	a
Producer gas turbine generator	Direct generation of electricity from producer gas generated from various biomass materials (Chapter 4; 7)			
Components Air Compressor			Gas : Air Ratio --> 1:5.14	[16]

			Air Bleed --> 13% Pressure = 20bar Polytropic Efficiency = 87% Mechanical Efficiency = 98%	[17]
Gas Compressor			Stages =3 Maximum stage temperature = 250°C Inter-stage cooling temperature = 97°C Pressure = 20bar Polytropic Efficiency = 80% Electric-Mechanical Efficiency = 90%	[18] [17]
Exhaust Gas Turbine			Turbine Isentropic Efficiency = 85% Turbine Electric-Mechanical Efficiency = 96%	[17]
Synthesis Gas Turbine generator	Electricity generated directly from unconverted syngas after methanol or FT synthesis (Chapter 6, 7).			

Components				
Air Compressor			Air added to affect an exhaust gas temperature of 650°C. Polytropic Efficiency = 87% Mechanical Efficiency = 96% Pressure = 22bar	
Exhaust Gas Turbine			Turbine Isentropic Efficiency = 85% Turbine Electric-Mechanical Efficiency = 96%	
Heat Recovery Steam Generator	Raises high pressure steam from producer gas (Chapter 4, 7), syngas and allothermal gasification stack gas (Chapter 6, 7), and turbine exhausts (Chapter 4, 6, 7).		HRSG Exit Gas Temperature (T) and Steam Pressure (SP) specified for: Producer Gas: T=97°C, SP = 60bar Syngas T=105oC; SP = 124bar Allothermal Gasification Stack: T=250°C; SP '=124bar Exhaust gas (BIGCC) = 250°C; SP = 60bar	[18] [17]

Steam Turbine Expansion			Exhaust gas (Synthetic Fuels) = 90°C; SP =124bar End steam pressure for sugar mill (Chapter 4,6) = 4bar End steam pressure for Sulphite mill (Chapter 5,7) '= 8bar Isentropic Efficiency =72% Turbine Electric-Mechanical Efficiency = 96%	[19] [3]
Biodigestion	20% reduction in Chemical Oxygen Demand of SSL	glucose --> 3 CH4 + 3 CO2 2 xylose --> 5 CH4 + 5 CO2 acetic acid --> CH4 + CO2 formic acid --> CO2 + H2	Temperature= 35°C Residence Time =	[20]

a. Reaction data from Cho et al.[21].
b. Plant conditions at Sappi Saiccor.

Table A 3: Synthetic Fuel Production Equipment

Unit Operations	Applicability and description	Reactions	Conditions	Reference/Note
Catalytic Allothermal Gasification	Gasification of sugarcane residues (Chapter 6) or bark (Chapter 7) in the presence of a dolomite catalyst for tar free syngas for synthetic fuel production.	Equilibrium Reactions	Moisture Content = 5% Steam to biomass ratio: 1:1 Proportion of Biomass Combusted = 42.0%	a.
Syngas Compression			Moisture Content = 5% Steam to biomass ratio: 1:1 Proportion of Biomass Combusted = 42.0% Stages: 3 stage pressure (CP), intercool temperature (IT) Stage 1: CP = 4.25bar; IT = 45°C Stage 2: CP = 17bar; IT = 45°C	[22]

			Stage 3: CP = 33bar	[23]
Rectisol Unit	Removal of acid gasses		CO2 removal = 97% H2S removal = 100%	[17]
			Electricity demand = 1.42kW/kmol syngas Heat demand = 7.57kW/kmol syngas	[23]
Methanol Reactors	Conversion of conditioned syngas gas to methanol either by conventional gas phase+recycle technology or advanced liquid phase technology	Equilibrium Reactions	Conventional Reactor Temperature = 300oC, Pressure = 60bar 87% of un-reacted gases recycled	[23]
			Advanced Reactor Temperature = 250oC, Pressure = 90bar	[24]
Fischer Tropsch Reactor	Conversion of conditioned syngas gas to FT syncrude either by conventional gas phase+recycle technology	3 H2 + CO --> CH4 + H2O 4 CO + 9 H2 --> C4H10	Conventional Reactor Temperature = 240°C, Pressure = 23.5bar	[25]

	or advanced slurry reactors	+ 4 H2O 9 CO + 19 H2 --> C9H20 + 9 H2O 15 CO + 31 H2 --> C15H32 + 15 H2O 21 CO + 43 H2 --> C21H44 + 21 H2O	40% conversion of CO per pass Molar Recycle Ratio. Mixed feed: Fresh Freed = 3:1 <u>Advanced Reactor</u> Temperature = 240°C, Pressure = 40bar 80% conversion of CO per pass	[26]

a. Gasification parameters obtained by optimisation

Table A 4: Utilities

Unit Operations	**Applicability and description**	**Reactions**	**Conditions**	**Reference/Note**
Cooling Tower	Used to cool cooling water to temperatures of 40oC throughout Chapter 4-7		Coefficient of performance = 11.95	[27]

Chiller	Maintains fermentation tanks at 30oC, Chapter 4,5,7		Coefficient of performance = 7	[28]

References

[1] Oliveira FMV, Pinheiro IO, Souto-maior AM, Martin C, Gonçalves AR, Rocha GJM. Industrial-scale steam explosion pretreatment of sugarcane straw for enzymatic hydrolysis of cellulose for production of second generation ethanol and value-added products. Bioresour. Technol. 2013;130:168–73.

[2] Rocha GJM, Martín C, Vinícius FN, Gómez EO, Gonçalves AR. Mass balance of pilot-scale pretreatment of sugarcane bagasse by steam explosion followed by alkaline delignification. Bioresour. Technol. 2012;111:447–52.

[3] Leibbrandt NH. Techno-Economics Study for Sugarcane Bagasse to Liquid Biofuels in South Africa: A Comparison between Biological and Thermochemical Process Routes. PhD Dissertation Department of Process Engineering. University of Stellenbosch, University of Stellenbosch 2010.

[4] Shevchenko SM, Chang K, Robinson J, Saddler JN. Optimization of monosaccharide recovery by post-hydrolysis of the water-soluble hemicellulose component after steam explosion of softwood chips. Bioresour. Technol. 2000;72:207–11.

[5] Nilverbrant N, Persson P, Reimann A, De Sousa F, Gorton L, Jonsson J. Limits for Alkaline Detoxification of Dilute-Acid Lignocellulose Hydrolysates. Applied Biochemistry and Biotechnology 2003;105-108:615–28.

[6] Alriksson B, Horvath I, Sjode A, Nilverbrant N, Jonsson L. Ammonium Hydroxide Detoxification of Spruce Acid Hydrolysates. Applied Biochemistry and Biotechnology 2005;121-124:911–22.

[7] Rudolf A, Baudel H, Zacchi G. Simultaneous Saccharification and Fermentation of Steam-Pretreated Bagasse Using Saccharomyces cerevisiae TMB3400 and Pichia stipitis CBS6054. Biotechnology and Bioengineering 2008;99:783–90.

[8] Kurian J., Minu A., Banerji A, Kishore VV. Bioconversion of hemicellulose hydrolysate of sweet sorghum bagasse to ethanol by using Pichia Stipitis NCIM 3497 and Debaryomyces Hansenii SP. Bioresources 2010;5:2404–16.

[9] Helle SS, Murray A, Lam J, Cameron DR, Duff SJB. Xylose fermentation by genetically modified Saccharomyces cerevisiae 259ST in spent sulfite liquor. Bioresour. Technol. 2004;92:163–71.

[10] Nigam JN. Ethanol production from wheat straw hemicellulose hydrolysate by Pichia stipitis. Journal of Biotechnology 2001;87:17–27.

[11] Humbird D, Davis R, Tao L, Kinchin C, Hsu D, Aden A, et al. Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol. National Renewable Energy Laboratory 2011.

[12] Dias MOS, Modesto M, Ensinas AV, Nebra SA, Maciel R, Rossell CEV. Improving bioethanol production from sugarcane : evaluation of distillation , thermal integration and cogeneration systems. Energy 2011;36:3691–703.

[13] Perin-Levasseur Z, Palese V, Marechal F. Energy integration study of a multi-effect evaporator. 11th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Prevention, 2008, pp. 1–17.

[14] Nsaful F. PROCESS MODELLING OF SUGAR MILL BIOMASS TO ENERGY CONVERSION PROCESSES AND ENERGY INTEGRATION OF PYROLYSIS. Stellenbosch University, 2012.

[15] Department of Tourism and Air Quality . AQA implementation: Listed activities and minimum emission standards. 2008.

[16] Uddin SN, Barreto L. Biomass-fired cogeneration systems with CO 2 capture and storage. Renewable Energy 2007;32:1006–19.

[17] Kreutz TG, Larson ED, Liu G, Williams RH. Fischer-Tropsch Fuels from Coal and Biomass. 25th Annual International Pittsburgh Coal Conference 2008.

[18] Craig KR, Mann MK. Cost and Performance Analysis of Biomass-Based Integrated Gasification Combined-Cycle (BIGCC) Power Systems Cost and Performance Analysis of Biomass-Based Integrated Gasification Combined-Cycle (BIGCC) Power Systems. National Renewable Energy Laboratory 1996.

[19] Nsaful F, Görgens JF, Knoetze JH. Comparison of combustion and pyrolysis for energy generation in a sugarcane mill. Energy Conversion and Management 2013;74:524–34.

[20] Jantsch TG, Angelidaki I, Schmidt JE, Brana de Hvidsten B., Ahring BK. Anaerobic biodegradation of spent sulphite liquor in a UASB reactor. Bioresour. Technol. 2002;84:15–20.

[21] Cho Y., Joseph B. Heterogeneous Model for Mowing-Bed Coal Gasification Reactors. Industrial Engineering Chemistry Process Design 1981;20:314–8.

[22] Phillips SD, Tarud JK, Biddy MJ, Phillips SD, Tarud JK, Biddy MJ. Gasoline from Wood via Integrated Gasification, Synthesis, and Methanol-to- Gasoline Technologies. 2011.

[23] Sun L, Smith R. Rectisol wash process simulation and analysis. J. Clean. Prod. 2013;39:321–8.

[24] Hamelinck CN, Faaij AP. Future prospects for production of methanol and hydrogen from biomass. 2001.

[25] Tijmensen MJ., Faaij AP., Hamelinck C., Van Hardeveld MRM. Exploration of the possibilities for production of Fischer Tropsch liquids and power via biomass gasification. Biomass Bioenerg. 2002;23:129–52.

[26] Ekbom T, Hjerpe C, Hermann F. Pilot study of Bio-jet A-1 fuel production for Stockholm-Arlanda Airport. Stockholm: 2009.

[27] Morvay ZK, Gvozdenac DD. Z. K. Morvay, D. D. Gvozdenac. Applied Industrial Energy and Environmental Management, John Wiley & Sons, Ltd; 2009, pp. 1–34.

[28] Smith BB. Economic Analysis of Hybrid Chiller Plants. 2002.

APPENDIX B: ECONOMIC INPUTS

In this appendix, the details and data on which the financial risk assessments of the various flow sheets are based are given. Firstly, the global parameters that describe the context in which the evaluations were completed are given. Thereafter, the procedure for calculating the total capital investment costs are given, which is based on values given in Table A 5 for the biological flow sheets and Table A 6 for synthetic fuel flow sheets. Thereafter, the procedures for simulating stochastic data using Monte Carlo methods is given, which is based on the data given in Table A 7. Finally, the financial modelling relating to the income statement, cash flow statement and balance sheet, and the calculation of Key Economic Indicators is given as equation format. Non-stochastic parameters and costs of chemicals are given Table A 8 and Table A 9, respectively. Thus, for the various journal article submissions, the procedures described, and the data that is applicable to the content of the chapters was given as supplementary/supporting information files.

1 Economic Assumptions

The parameters under which the economic evaluations of the scenarios were carried out are as follows:

- To simplify the economic analysis, an equity pool is assumed.
- The life of the plant is 25 years and the period of analysis is 20 years.
- The plant will have a salvage value of 20%, and the depreciation will be determined linearly from the initial value of the plant to the salvage value.
- Operational time for Chapter 4 and 6 is 6400 hours and 8000 hours for Chapters 5 and 7.
- The South African Company Tax rate of 28% applies.
- The working capital is 5%

2 Capital Cost Estimation

2.1 EQUIPMENT COSTS

1. The capital cost of major equipment was estimated from literature using Equation 1. The values of the parameters in Equation 1 Table A 5 for the biological flow sheets and Table A 6 for synthetic fuel flow sheets

$$C_{ME} = RC*(SP_S/SP_R)^{SF}*IF*(CEPCI_{FY}/CEPCI_{RY})$$

Where C_{ME} – Capital Estimation of Major Equipment

RC – Reference quoted price

SP – Scaling Parameter, simulated (S) and reference value (R).

SF – Scaling Factor

IF- Installation Factor

CEPCI – Chemical Engineering Plant Cost Index, of the first year of analysis (FY), and reference year (RY).

2. Aspen Icarus[1] was used to estimate the costs of generic equipment (C_{GE}) such as pumps, turbines, compressors, flash tanks and process heaters and coolers.

3. The Total Equipment Costs (TEC)

$$TEC = \sum C_{ME} + \sum C_{GE}$$

4. The Balance of Plant (BOP) [2], which estimates the costs of piping, instrumentation and wiring, is then calculated as:

$$BOP\ (\%) = 0.8867 / (\text{Biomass Higher Heating Calorific Input (MW)})^{0.2096}$$

5. The Total Installed Costs (TIC) are calculated as:

   TIC = TEC+BOP+SD+W

   Where: SD – Site Development, 13.5% of TEC [3]

   W – Warehouses, 1.5% of TEC [3]

6. Total Fixed Costs (TFC) is calculated as

   TFC = PC + FE +OC + C + O + TIC

   Where: PC – Prorateable Costs

   FE – Field Expenses, 10% of TFC [3]

   OC – Office and Construction, 20% of TFC [3]

   C – Contingency 10% of TFC [3]

   O – Other Costs 10% of TFC [3]

7. Finally, the Total Investment Capital (TC) is calculated as

   TC = TFC+WC

   Where, WC – Working Capital, 5% of TFC. [3]

8. A location factor of 0.90 relative to a USA value of 1 is assumed on the Total Investment Capital [4].

Table A 5: Parameters for Equipment Capital Estimate for Bioethanol Production (Chapter 4, 5, 7)

Unit	Scale Parameter	Base Value USD	Base Year	Base Price	Base CEPCI	Scale Factor	Installation
Hemicellulose Extraction[3]	ton/h wet biomass	83.3	2010	6604149	560	0.6	1.5
Oligomer Hydrolysis[3]	kg/hr Hydrolysate	292060	2010	203000	560	0.7	2
Detoxification Reactor[5]	kg/hr Hydrolysate	268762	2000	100144	392	0.71	1.40
Neutralisation Reactor[5]	kg/hr Hydrolysate	268762	2000	100144	392	0.71	1.40
Filter Press[5]	t/h solids	21	2000	1 285 736	392	0.60	2.40
Seed Fermenters' Coil[5]	Heat Duty	245	1997	4658	387	0.83	1.20
Seed Fermenters[6]	Volume m3	727	2000	149345	392	0.51	1.20
Seed Holding Tank[6]	Volume m3	872	2000	175626	392	0.51	1.20
Fermentation Cooler[5]	Heat Duty	2800	1997	3054	387	0.78	2.10
Fermentation Tank[6]	Volume m3	3596	2000	539848	392	0.51	1.20
Water scrubber[6]	kg/h total feed	25325	2000	127848	392	0.78	2.75
Distillation columns[3]	t/h ethanol	29	2010	3327914	560	0.60	2.40
Molecular sieve[3]	t/h ethanol	22	2010	2920000	560	0.60	1.80
Boiler	t/h steam	100	2010	31250000	560	0.73	1.00
Heat Exchangers[7]	Area m2	167	2010	44200	560	0.68	2.86
Digester[8]	m3	1	2010	714	560	0.91	1.00

Chiller[9]	Heat Duty kW	1	2002	299	396	0.80	1.00
Bag-house[5]	Kmol Flue gas	12935	2000	1784255	392	0.58	1.50
BIGCC Plant[10]	tons/day dry biomass	452	2007	39 458 000	525	0.6	1

Table A 6: Parameters for Equipment Capital Estimate for Synthetic Fuel Production (Chapter 6, 7)

Item	Parameter		Base Capacity	Cost (2012)	Factor	Installation
Biomass Dryer[11]	kg/hr Water Removed	kg/hr	1	334	1.00	1.00
Shredder[5]	ton/hr biomass	ton/hr	42	19 100 119	.70	1
Dual Fluidised Bed Reactor[12]	ton/hr biomass	ton/hr	42	19 100 119	0.70	1.00
CFB Reactor[12]	ton/hr biomass	ton/hr	42	12 513 922	0.70	1.00
Pressurised Gasification[12]	ton/hr biomass	ton/hr	42	17 835 175	0.70	1.00
Air Separation Unit[13]	O2 Flow kg/s	kg/s	64800	36 711 538	0.50	1.00
Rectisol Unit[2]	m3/h syngas	Nm3/hr	200000	31 392 767	0.63	1.32
Compressor[2]	KW	kW	70000	6 878 068	0.67	1.32
Methanol Synthesis - Conventional[14]	Methanol Product	ton/hr	88	10 167 132	0.60	2.10
Heat Recovery Steam Generator[2]	Heat Load	MW	355	56 681 386	1.00	1.27
Distillation[15]	Methanol Product	ton/hr	87	18 684 256	0.67	1.00
Surface Condenser[16]	Heat Duty	MW	498	47 461 940	0.68	1.00
Vacuum Pump[17]	Flow	m3/s	13	283 954	0.79	2.80
Cooling Tower[5]	Heat Duty	kW	618903	2 439 305	0.78	1.20

Electric Boiler	Load	kW	3600	107 811	0.80	1.00
Bag Filter[18]	Flow	m3/s	12	2 323 916	0.65	1.86
Gas Turbine[2]	Gross Generation	MW	150	66 166 311	0.75	1.27
Methanol Synthesis - Advanced[14]	Methanol Product	ton/hr	88	5 083 566	0.72	2.10
Auto-Thermal reformer[2]	Input	MM SCF/day	365	32 591 797	0.67	1.32
FT Reactor - Advanced[2]	FT Input Volume	MM SCF/hr	3	14 824 362	0.75	1.32
FT Reactor -Conventional[18]	FT Liquid energy	MW	100	24 398 189	1.00	1.00

Table A 7: Data for Stochastic Variables in Economic Models

	USA ethanol[19, 20]	Brazilian ethanol[21]	Electricity[22]	Methanol[23]	Crude[24]	PPI[25]	Interest Rates[26]
			kWhr	$ per litre	$ per litre		
2003	0.337	0.252	0.032	0.202	0.181	124.8	15.16
2004	0.422	0.254	0.039	0.208	0.240	127.7	11.31
2005	0.463	0.375	0.044	0.234	0.342	132.4	10.64
2006	0.674	0.508	0.048	0.296	0.410	142.6	11.14
2007	0.524	0.467	0.040	0.346	0.456	158.2	13.08
2008	0.587	0.520	0.040	0.435	0.610	180.8	15.12
2009	0.449	0.450	0.045	0.198	0.387	180.7	11.80
2010	0.483	0.612	0.054	0.274	0.500	191.6	9.91

2011	0.683	0.867	0.087	0.346	0.700	207.6	9.00
2012	0.611	0.666	0.106	0.351	0.702	220.5	8.78

PREPARATION OF STOCHASTIC SIMULATION

The method described here is a summary of the method found in Richardson et al[27], and Amigun et al[28].

1. The raw data for stochastic variables (i) in Table A 7 is used to derived time dependant linear equations, or an average valued indices, where from future values can be projected from

$$TDTV_{i\ (t=2003\ldots2012))}=m_i \cdot t+c_i$$

or

$$EV_{i\ (t=2003,2012)}=Average_i\ (t=2003\text{-}2012)$$

Where: TDTV - time dependant trend value
m&c - trend line gradient and intercept.
EV - expected value

2. The residuals associated with each historical data point for each variable (Res_i) will be calculated as the difference between the measured variable and its associated trend/expected value

Thus: $$Res_{i,\ (t=2003\ldots2012)}=MHV_{i(t)} - TDTV_{i(t)}$$

OR

$$Res_{i,\ (t=2003\ldots2012)}=MHV_{i(t)} - EV_{i(t)}$$

Where: MHV - measured historic value

3. The relative variances (V) associated with each residual and the trended value will be calculated as:

$$V_{i\ (t=2003\ldots.2012)}=Res_{i(t)}/TDTV_{i(t)}$$

OR

$$V_{i\,(t=2003....2012)}=Res_{i(t)}/EV_{i(t)}$$

4. The multivariate empirical distribution (MVEMP) characterising the measured variances will be used to simulate a vector of simulated variances (SV).

   Thus: $\{SV_i\}_{t=2012...2031}=MVEMP(V_{i,\,t=2003...2012})$

5. Future yearly values will be simulated either as future time dependant trend value (FTDTV) or future expected values (FEV) using the formulas determined for the trend lines in Step (1)

$$FTDTV_{i\,,t=2012...2031}=TDTV_{,i\,,t=2012...2031}$$

OR

$$FEV_{i,\,t=2012...2031}=EV_{i,\,t=2003...2012}$$

6. The simulated future variance will then be combined with the future yearly value to calculated the stochastic Forecasted Economic Input (SFI).

$$SFI_{i,\,,t=2012...2031}=FTDTV_{i,\,t=2012...2031}+FTDTV_{i,\,t=2012...2031}*SV_{i,\,t=2012...2031}$$

OR

$$SFI_{i,\,,t=2012...2031}=FEV_{i,\,t=2012...2031}+FEV_{i\,,t=2012...2031}*SV_{i,\,t=2012...2031}$$

7. Simulation of the Operating time (T) would be accomplished with the GRKS distribution with a 10 day variation around the average operating time of 8000 hours.

   Thus T=GRKS(7760, 8000, 8240)

Table A 8: Static Inputs for Economic Models

Sugarcane Trash[29]	US$/ton	20.44
Natural Gas[24]	US$/ton	893.00

O&M Costs: Ethanol Production (Chapter 4,5,7)	US$/litre	0.032
Added Maintenance Costs of Recovery Boiler[a] (Chapter 5,7)	US$/litre	0.003
CHPSC Operating Costs[10]	US$/litre	0.007
BIGCC Operating Costs[10]	US$/litre	0.013
O&M Costs: Methanol Synthesis[30]	US$/ton biomass	23.17
O&M Costs: FT Synthesis[31]	US$/ton biomass	25.63

Estimated as the running costs of maintaining the bag-house filter that captures ash[3].

SUMMARY OF FINANCIAL MODEL FOR CALCULATING THE KEY ECONOMIC VARIABLES

1. Simulating the Operating Expenses (OE) or Operating Incomes (OI)

   If stochastic (i): $OI_{i,t}$ or $OE_{i,t}$ = Flow $rate_i$*T*$SFI_{i,t}$

   If not stochastic (j) : $OE_{j,t}$ = Base $value_j$ *$SFI_{PPI,t}$/$PPI_{t=2012}$

2. Interest Calculations

   Accrued $Interest_t$ = (Negative cash balance)$_{t-1}$*$SFI_{interest}$

   Interest $Earned_t$ = (Positive cash balance)$_{t-1}$*Interest on Positive Bank Balance

3. Net $Profit/loss_t$ = $\sum OI_{i,t}$ + Interest $Earned_t$ - $\sum OE_{i,t}$ – Accrued $Interest_t$

   NOTE: In South Africa, tax is paid on interest earned at these scales. Please see the SARS website for further information.

4. Net Cash Income/Deficit = Net $Profit/loss_t$ – $Depreciation_t$.
5. $Dividends_t$ = Net $Income_t$ * 25%
6. Tax_t=Net $Income_t$*28%
7. Cash $Flow_t$ = Net Cash $Income_t$ - Tax_t - $Dividends_t$ OR = Net Cash Deficit
8. Cash $Balance_t$ = Cash $Balance_{t-1}$ + Cash $Flow_t$
9. $Assets_t$ = Plant $Value_{t-1}$-$Depreciation_t$+Land Value + Cash $Balance_t$ (IF >0)
10. Liabilities = IF Cash $Balance_t$ <0, Cash $Balance_t$, else = 0
11. Owners $Equity_t$ = $Assets_t$ – $Liabilities_t$
12. Delta Net $Worth_t$ = Owners $Equity_t$ - Owners $Equity_{t-1}$
13. Present $Value_t$ = (Delta Net $Worth_t$ + $Dividends_t$)/(1+Discount $Rate_{(=12.64\%)}$)^t
14. Net Present Value = -Total Capital Investment (TIC)+$\sum$Present Values
15. For IRR – Solve for the discount Rate to yield a zero Net Present Value

Table A 9: Quotes for chemical costs used in bioethanol production (Chapter 4, 5, 7)

Chemical	Price	Unit	Year	Source	PPI	USD/kg	USD/kg
					reported year		2012
Sulphur	180	USD/m3	2006	1	142.6	0.087	0.134
Nitric Acid	215	USD/ton	2006	1	142.6	0.215	0.332
Ammonium Hydroxide	460	USD/ton	2007	1	154.85	0.460	0.655
Hydrochloric Acid	93.7	USD/ton	2010	1	191.6	0.094	0.145
Sulphuric Acid	200	USD/ton	2010	2	191.6	0.200	0.285
Molasses	184	USD/ton	2012	3	220.5	0.184	0.184
Sodium Hydroxide	850	USD/ton	2006	1	142.6	0.937	1.449
Corn Steep Liquor	177	USD/ton	2010	2	191.6	0.100	0.115
Ammonium Sulphate	335	USD/ton	2006	1	142.6	0.189	0.293
Di-ammonium Phosphate	230	USD/ton	2006	1	142.6	0.130	0.201
Ammonia	521	USD/ton	2006	1	142.6	0.295	0.455
Potassium Dihydro-Phosphate	41.25	USD/100lb	2006	1	142.6	0.909	1.406
Unrefined sugar	0.131	cent/pound	2010	3	191.6	0.289	0.332
Magnesium Sulphate	21	USD/lb	2006	1	142.6	0.463	0.716

3 References

1. Aspen Technology Inc: **Aspen Plus®, Aspen Icarus®**. 2008.

2. Kreutz TG, Larson ED, Liu G, Williams RH: **Fischer-Tropsch Fuels from Coal and Biomass**. *25th Annual International Pittsburgh Coal Conference* 2008(August).

3. Humbird D, Davis R, Tao L, Kinchin C, Hsu D, Aden A, Schoen P, Lukas J, Olthof B, Worley M, D. Sexton and DD: **Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol**. *National Renewable Energy Laboratory* 2011(May).

4. Perry RH, Green DW: *Perry's Chemical Engineers' Handbook McGraw-Hill*. 7th Editio. Handbook McGraw-Hill; 1997.

5. Aden A, Ruth M, Ibsen K, Jechura J, Neeves K, Sheehan J, Wallace B, Montague L, Slayton A, Lukas J: **Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis for Corn Stover Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehyd**. *National Renewable Energy Laboratory* 2002(June).

6. Leibbrandt NH: **Techno-Economics Study for Sugarcane Bagasse to Liquid Biofuels in South Africa: A Comparison between Biological and Thermochemical Process Routes**. *PhD Dissertation Department of Process Engineering University of Stellenbosch, University of Stellenbosch* 2010.

7. Al-Riyami BA, Klimes J, Perry S: **Heat Integration reftrofit analysis of a heat exchanger network of a fluid catalytic cracking plant**. *Applied Thermal Engineering* 2001, **21**:1449-1487.

8. Zamalloa C, Vulsteke E, Albrecht J, Verstraete W: **Bioresource Technology The techno-economic potential of renewable energy through the anaerobic digestion of microalgae**. *Bioresour Technol* 2011, **102**:1149-1158.

9. He B, Setterwall F: **Technical grade paraffin waxes as phase change materials for cool thermal storage and cool storage systems capital cost estimation**. *Energy Conversion and Management* 2002, **43**:1709-1723.

10. U S Environmental Protection Agency: *Biomass Combined Heat and Power Catalog of Technologies*. 2007(September).

11. Amos WA: *Report on Biomass Drying Technology Report on Biomass Drying Technology*. 1998(November).

12. Worley M, Yale J: *Biomass Gasification Technology Assessment Consolidated Report Biomass Gasification Technology Assessment Consolidated Report*. 2012(November).

13. Larson ED, Jin H, Celik FE: **Large-scale gasification-based coproduction of fuels and electricity from switchgrass**. *Biofuels Bioproducts and Refining* 2009, **3**:174-194.

14. Hamelinck CN, Faaij AP.: *Future Prospects for Production of Methanol and Hydrogen from Biomass*. 2001(September).

15. Dijk KM van, Dijk R van, Eekhout VJL van, Hulst H van, Schipper W, Stam JH, Rllemkens J, Badger B.V. DH, Grievink J, Llteijn CP, Meijer FA: *Methanol from Natural Gas: Conceptual Design & Comparison of Processes*. Delft; 1995.

16. Ridgway S.: **Projected Capital Costs of a Mist Lift OTEC Power Plant**. *The American Society of Mechanical Engineers* 1984.

17. Bailey D: **Issues Analysis of Retrofitting Once-Through Cooled Plants with Closed-Cycle Cooling**. *Electric Power Research Institute (USA)* 2007.

18. Tijmensen MJ., Faaij AP., Hamelinck C., Van Hardeveld MRM: **Exploration of the possibilities for production of Fischer Tropsch liquids and power via biomass gasification**. *Biomass Bioenerg* 2002, **23**:129–152.

19. **Official Website** [http://www.neo.ne.gov/statshtml/66.html]

20. **Ethanol Prices** [www.card.iastate.edu]

21. **CEPEA** [http://www.cepea.esalq.usp.br/xls/SaaofmensalUS.xls]

22. **Eskom Tariffs and Charges** [www.eskom.co.za/content]

23. **Methanol Prices**
[https://www.methanex.com/products/documents/MxPriceSheetJanuary292014.pdf]

24. Matseba L, Nembahe R: *SOUTH AFRICAN ENERGY Price Report 2012*. Pretoria; 2012.

25. **Producer Purchases Index** [www.statsa.gov.za/keyindicators/ppi]

26. **Reserve Bank, Historical Exchange and Interest Rates** [http://www.resbank.co.za/Research/Rates/Pages/SelectedHistoricalExchangeAndInterestRates.aspx]

27. Richardson JW, Lemmer WJ, Outlaw JL: **Bio-ethanol Production from Wheat in the Winter Rainfall Region of South Africa : A Quantitative Risk Analysis**. *Int Food Argibus Manag Rev* 2007, **10**:181-204.

28. Amigun B, Petrie D, Görgens J: **Economic risk assessment of advanced process technologies for bioethanol production in South Africa : Monte Carlo analysis**. *Renewable Energy* 2011, **36**:3178-3186.

29. Petersen AM, Aneke M, Gorgens JF: **Techno-economic comparison of ethanol and electricity coproduction schemes from sugarcane residues at existing sugar mills in Southern Africa**. *Biotechnol Biofuel* 2014, **7**:1-19.

30. Ren T, Daniëls B, Patel MK, Blok K: **Petrochemicals from oil, natural gas, coal and biomass: Production costs in 2030–2050**. *Resources, Conservation and Recycling* 2009, **53**:653-663.

31. Ekbom T, Hjerpe C, Hermann F: *Pilot Study of Bio-jet A-1 Fuel Production for Stockholm-Arlanda Airport*. Stockholm; 2009.

APPENDIX C: GREENHOUSE GAS INVENTORY

In this appendix, the data of the inventory for the Greenhouse Gas calculations in Chapters 5 and 7 is given. Tables A1 to A3 shows the data and the references or derivation of the numbers given are described in footnotes.

Table A 10: Emissions Per ton of Coal Used

Mining Emission			Reference/ Note
Methane Emissions per ton of Coal	0.50	m3/ton	[1]
Density of methane	0.68	kg/m3	Average density between 0 and 25°C
Thus	0.34	kg/ton	
CO2 Eq	8.50	kg/ton	a
Coal Transport			
GHG Transport of coal	0.20	kg/km	[2]
Distance	600.00	km	b
Tons per Trip	45.00	tons	b
Coal Combustion (per ton)	2.97	ton CO2 eqt	c

a. Calculated using the methane GWP equivalent of 25[3].

b. Information provided by Sappi Saiccor personnel.

c. Extracted from SimaPro[4] database, as generated by the CML2000 method.

Table A 11: Greenhouse Gas associated with Chemicals

	kg CO2 eqt	Reference/ Note
Hydrochloric Acid	0.85	a, b
Sodium Hydroxide	1.41	a
Glucose	0.01	a
Corn Steep Liquor	1.90	c
Ammonia	2.40	A
Magnesium Sulphate	0.30	A
Di-ammonium Phosphate	2.81	A
Ammonium Sulphate	2.70	A

a. Extracted from SimaPro[4] database, as generated by the CML2000 method.

b. Hydrochloric acid or sulphuric acid used as possible acidifying agents.

c. Estimated from the energy balance of the Steeping Process[5], using the emissions for coal given in Table A 10.

Table A 12: Avoidance of fossil transport fuel GHG with Biofuels

Biofuel	kg CO2 eqt/l	Reference/ Note
Ethanol	1.57	a
Methanol	1.56	b
FT Syncrude	2.21	c

a. Based on the displacement of tail pipe greenhouse gas emission of fossil gasoline (based on the emission values extracted from the GREET[2] model) by the use of bioethanol, on an thermal energy basis.

b. Based on the reduction of tail pipe greenhouse gas emission of Biodiesel 20 (based on the emission values extracted from the GREET[2] model), if the fossil based methanol used in the biodiesel process is replaced by biomethanol. The contribution of methanol to the greenhouse gas emission of the production life-cycle of biodiesel was calculated at 9.6%, based on data given by Elsayed et al[6] .
c. Based on the Based on the displacement of tail pipe greenhouse gas emission of fossil gasoline in a passenger car and diesel in a truck(based on the emission values extracted from the GREET[2] model), assuming these fuels are alternatively originated from bio-syncrude.

References

[1] Zhou PP, Lloyd P, Mzezewa C, Kipondya F, Asamoah J, Simonsen H. Determination of regional emission factors for the power sector in Southern Africa. Journal of Energy in Southern Africa 2009;20:11–8.

[2] Wang M, Burnham A, Wu Y. GREET 2007.

[3] Shindell DT, Faluvegi G, Koch DM, Schmidt GA, Unger N, Bauer SE. Improved Attribution of Climate Forcing to Emissions. Science 2009;326.

[4] PRé-Consultants. SimaPro 2010.

[5] Galitsky C, Worrell E, Ruth M. Energy Efficiency Improvement and Cost Saving Opportunities for the Corn Wet Milling Industry An ENERGY STAR Guide for Energy and Plant Managers. California: 2003.

[6] Elsayed MA, Matthews R, Mortimer ND. CARBON AND ENERGY BALANCES FOR A RANGE OF BIOFUELS OPTIONS. 2003.

APPENDIX D: PROCESS FLOW-SHEETS AND STREAM DATA

In this thesis, a total of 34 scenario flow-sheets were developed and analysed, with each flow sheet having several subsections that serves as common “component flow-sheets” to the flow sheets of the scenario in the various chapters. Thus, in this appendix, only the mass balances around the subsection flow-sheets will be displayed in order to avoid redundant representations of the same subsections. Tables A1-A4 demonstrates how the various subsections are connected to form the main flow sheets analysed in the chapters of this study. For sections A1-A3, at least one scenario will have a complete mass balance represented since all the subsections are shown.

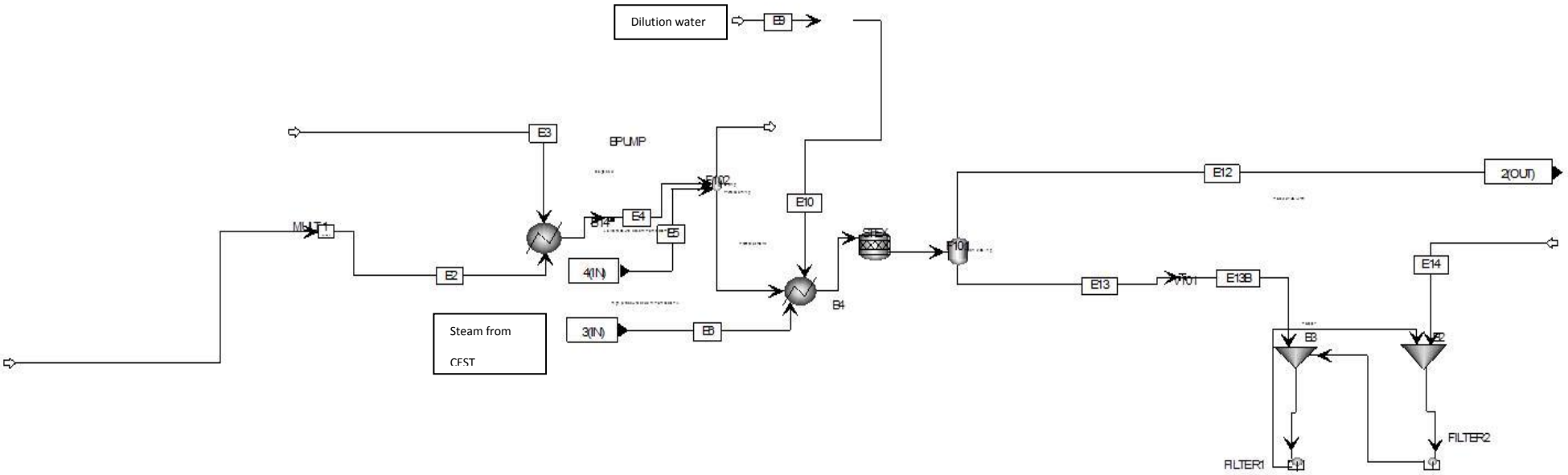
1. APPENDIX D1

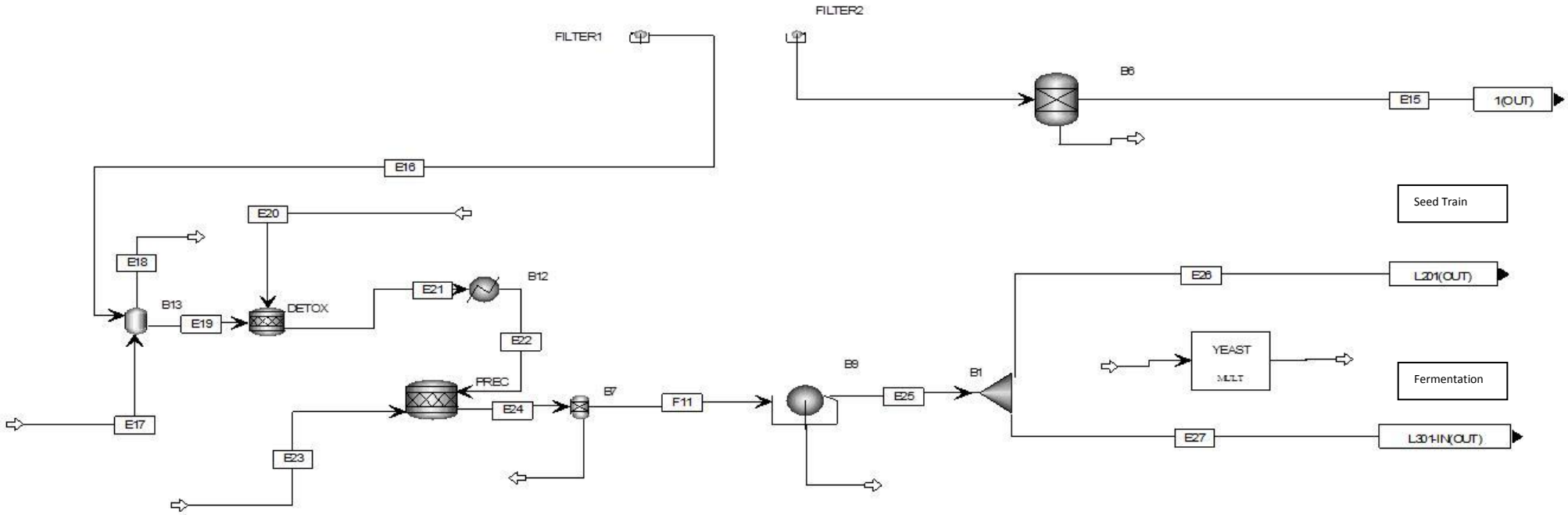
Table D 13: Configuration of flow sheets for Chapter 4: (CPE – Co-production of ethanol and electricity; CON – conventional distillation; VAC – vacuum distillation; BIGCC – Biomass integrated gasification and combined cycles; CHPSC – Combustion with high-pressure steam cycles; -EE- Exclusive Electricity production)

Overall Scenarios		Subsections/Component flow-sheets								
		Hemicellulose Extraction and Detoxification	Seed Train	Fermentation	Vacuum Distillation	Conventional Distillation	CHPSC - CPE	BIGCC - CPE	CHPSC - EE	BIGCC - EE
Flow Sheets	CPE-CON-BIGCC*	X	X	X		X		X		
	CPE-VAC-BIGCC*	X	X	X	X			X		
	CPE-CON-CHPSC*	X	X	X		X	X			
	CPE-VAC-CHPSC*	X	X	X	X		X			
	CHPSC – EE*								X	
	BIGCC – EE*									X

*full mass balance represented

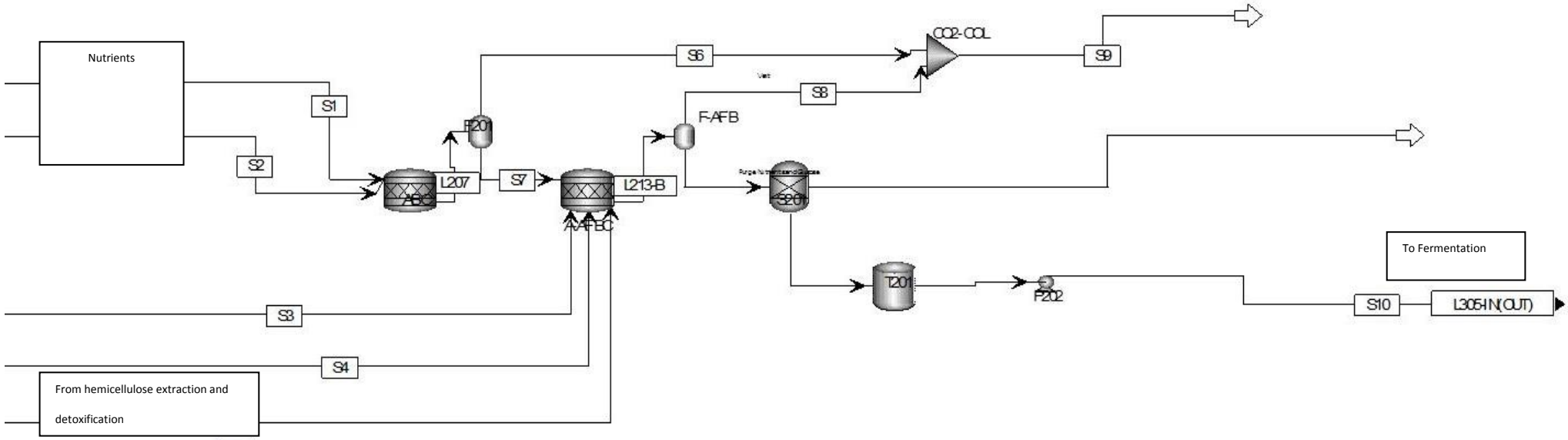
1.1 HEMICELLULOSE EXTRACTION AND DETOXIFICATION





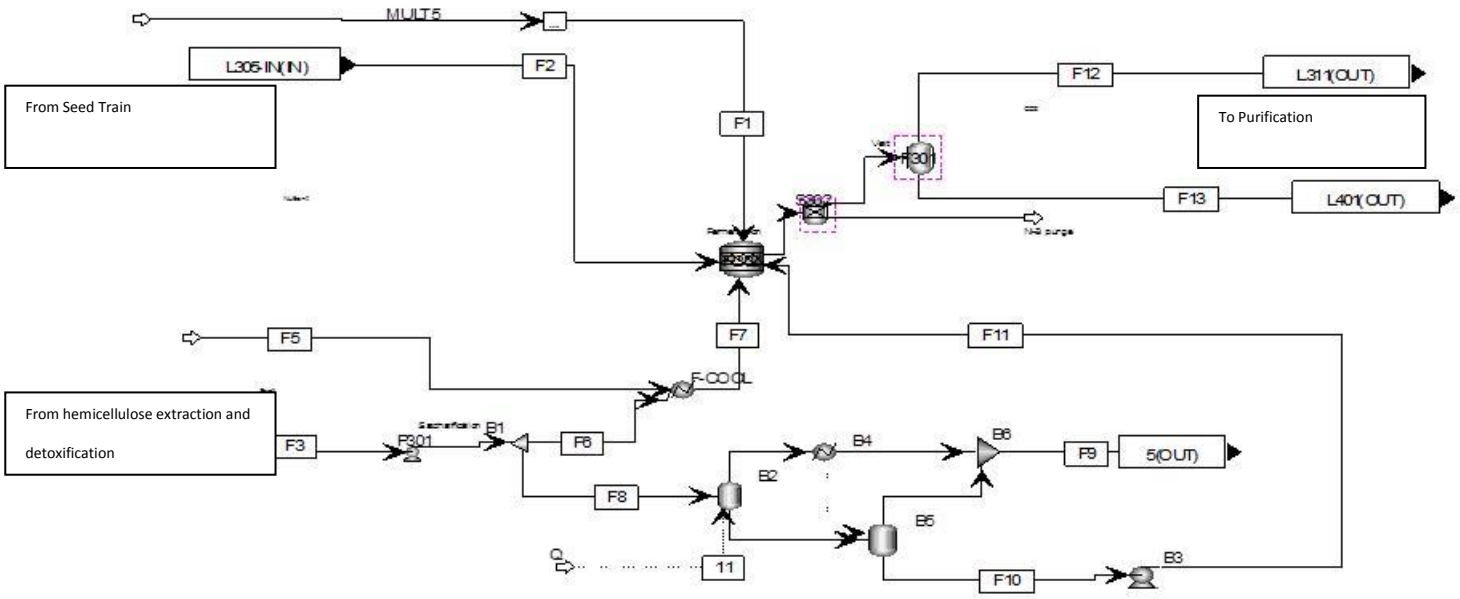
	E1	E2	E3	E4	E5	E6	E8	E9	E10	E11	E12	E13	E13B	E14	E15	E16	E17	E18	E19	E20	E21	E22
Substream: MIXED																						
Mass Flow kg/hr																						
GLUCOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4548.1	0.0	4548.1	4548.1	0.0	905.3	3642.8	0.0	0.0	3642.8	0.0	3642.8	3642.8
XYLOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15889.0	0.0	15889.0	15889.0	0.0	3162.6	12726.4	0.0	0.0	12726.4	0.0	12726.4	12726.4
ARABINOS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1172.8	0.0	1172.8	1172.8	0.0	233.4	939.4	0.0	0.0	939.4	0.0	939.4	939.4
GALACTOS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	474.1	0.0	474.1	474.1	0.0	94.4	379.8	0.0	0.0	379.8	0.0	379.8	379.8
MANNOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	105.4	0.0	105.4	105.4	0.0	21.0	84.4	0.0	0.0	84.4	0.0	84.4	84.4
CELLOB	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	178.1	0.0	178.1	178.1	0.0	35.5	142.7	0.0	0.0	142.7	0.0	142.7	142.7
EXTRACT	75.0	3150.0	1506.1	4656.1	0.0	0.0	0.0	0.0	0.0	4656.1	0.0	4656.1	4656.1	0.0	926.8	3729.3	0.0	0.0	3729.3	0.0	3729.3	3729.3
H2O	1000.0	42000.0	4000.6	46000.6	6425.1	16205.3	266.2	15000.0	15000.0	80783.4	18031.9	62751.6	62751.6	35298.9	34573.8	63476.6	0.0	0.0	63476.6	0.0	63635.0	63635.0
AACID	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1148.3	158.1	990.2	990.2	0.0	197.1	793.1	0.0	0.0	793.1	0.0	793.1	793.1
FURFURAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	358.2	13.5	344.7	344.7	0.0	68.6	276.1	0.0	0.0	276.1	0.0	276.1	276.1
H2SO4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	431.0	0.0	431.0	0.0	0.0	0.0
NH4OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	342.6	17.0	17.0
Total Flow kmol/hr	55.9	2347.6	229.8	2577.4	356.6	899.5	14.8	832.6	832.6	4674.1	1003.7	3670.4	3670.4	1959.4	1956.4	3673.4	4.4	0.0	3677.8	0.0	3682.2	3682.2
Total Flow kg/hr	1075.0	45150.0	5506.7	50656.7	6425.1	16205.3	266.2	15000.0	15000.0	109314.0	18203.5	91110.1	91110.1	35298.9	40218.5	86190.5	431.0	0.0	86621.5	0.0	86348.9	86348.9
Total Flow l/min	16.8	706.5	69.0	798.5	51338.8	36567.8	6323.0	250.7	258.1	1912.1	516775.0	1423.9	1423.9	609.6	680.9	1368.8	4.0	0.0	1394.5	0.0	80512.4	1320.2
Temperature K	298.2	298.2	298.2	358.2	424.1	581.3	378.6	298.2	358.2	473.2	374.2	374.2	374.2	363.2	366.1	372.4	298.2		393.2	298.2	374.3	303.2
Pressure bar	1.0	1.0	1.0	4.3	4.0	19.0	1.2	1.0	1.0	19.5	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.9	1.9	1.0	1.0	1.0
Vapor Frac	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0		0.0		0.0	0.0
Liquid Frac	1.0	1.0	1.0	1.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0		1.0		1.0	1.0
Solids																						
Mass Flow kg/hr																						
CELLULOS	406.0	17052.0	9666.8	26718.8	0.0	0.0	0.0	0.0	0.0	22465.2	0.0	22465.2	22465.2	0.0	22465.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLAN	231.0	9702.0	6187.1	15889.1	0.0	0.0	0.0	0.0	0.0	403.6	0.0	403.6	403.6	0.0	403.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LIGNIN	216.0	9072.0	5464.9	14536.9	0.0	0.0	0.0	0.0	0.0	14536.9	0.0	14536.9	14536.9	0.0	14536.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARABINAN	20.0	840.0	490.0	1330.0	0.0	0.0	0.0	0.0	0.0	297.9	0.0	297.9	297.9	0.0	297.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MANNAN	2.0	84.0	49.0	133.0	0.0	0.0	0.0	0.0	0.0	38.2	0.0	38.2	38.2	0.0	38.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GALACTAN	9.0	378.0	220.5	598.5	0.0	0.0	0.0	0.0	0.0	171.8	0.0	171.8	171.8	0.0	171.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH	41.0	1722.0	582.9	2304.9	0.0	0.0	0.0	0.0	0.0	2304.9	0.0	2304.9	2304.9	0.0	2304.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	7.0	292.6	166.8	459.4	0.0	0.0	0.0	0.0	0.0	304.9	0.0	304.9	304.9	0.0	304.9	0.0	0.0	0.0	0.0	4.6	4.6	4.6
Total Flow kg/hr	925.0	38850.0	22661.2	61511.2	0.0	0.0	0.0	0.0	0.0	40218.5	0.0	40218.5	40218.5	0.0	40218.5	0.0	0.0	0.0	0.0	342.6	615.2	615.2
Total Flow l/min	11.3	474.8	278.5	761.9	0.0	0.0	0.0	0.0	0.0	526.7	0.0	514.1	514.1	0.0	513.1	0.0	0.0	0.0	0.0	2.5	3.5	3.5
Temperature K	298.2	298.2	298.2	358.2						473.2		374.2	374.2		366.1					298.2	374.3	303.2
Pressure bar	1.0	1.0	1.0	4.3	4.0	19.0	1.2	1.0	1.0	19.5	1.0	1.0	1.0	1.0	1.0		1.0	1.9	1.9	1.0	1.0	1.0

1.2 SEED TRAIN



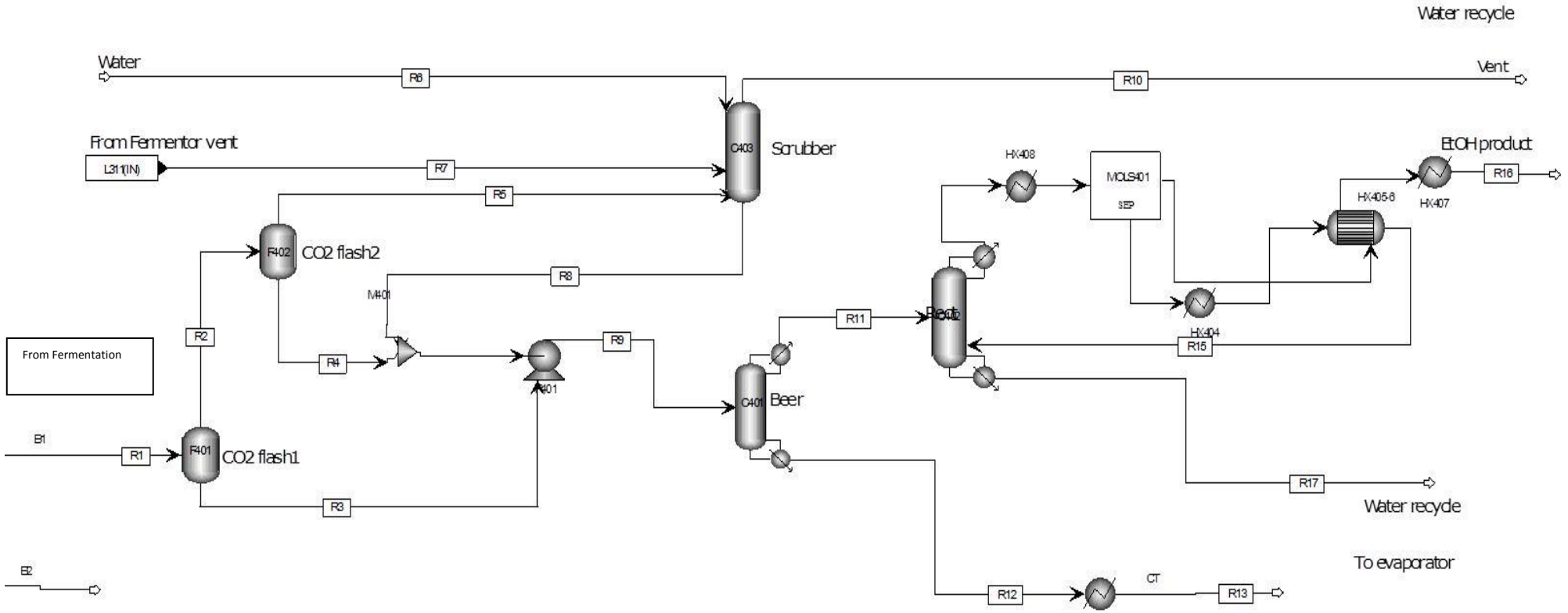
	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
Substream: MIXED										
Mass Flow kg/hr										
GLUCOSE	1.3	0.0	0.0	28.8	27.3	0.0	0.0	0.0	0.0	0.0
XYLOSE	0.0	0.0	0.0	100.7	82.0	0.0	0.0	0.0	0.0	0.0
ARABINOS	0.0	0.0	0.0	7.4	0.0	0.0	0.0	0.0	0.0	7.4
GALACTOS	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	3.0
MANNOSE	0.0	0.0	0.0	0.7	0.0	0.0	0.0	0.0	0.0	0.7
CELLOB	0.0	0.0	0.0	1.1	0.0	0.0	0.0	0.0	0.0	1.1
CSL	0.0	0.0	0.0	29.5	20.5	0.0	0.0	0.0	0.0	0.0
ETHANOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	0.0	0.0	0.0	503.6	1.0	0.2	0.3	35.9	36.1	540.7
N2	0.0	5.1	1027.6	0.0	0.0	5.1	0.0	1027.6	1032.8	0.0
CO2	0.0	0.0	0.0	0.0	0.0	1.3	0.0	175.0	176.3	0.1
O2	0.0	1.5	289.8	0.0	0.0	0.5	0.0	162.6	163.1	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LACID	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
AACID	0.0	0.0	0.0	6.3	0.0	0.0	0.0	0.2	0.2	6.0
GLYCEROL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NUTRIENT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARGON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURAL	0.0	0.0	0.0	2.2	0.0	0.0	0.0	0.0	0.0	2.2
KH2PO4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MGSO4-01	0.0	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.0
(NH4)2SO4	0.0	0.0	0.0	0.0	0.7	0.0	0.0	0.0	0.0	0.0
(NH4)3PO4	0.0	0.0	0.0	0.0	1.4	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	0.0	0.2	45.7	29.1	0.9	0.2	0.0	47.7	48.0	30.2
Total Flow kg/hr	1.3	6.6	1317.5	683.4	133.2	7.1	0.3	1401.3	1408.5	561.2
Total Flow l/min	0.0	93.4	18642.4	10.2	1.5	99.1	0.0	19772.8	19871.9	9.3
Temperature K	303.2	298.2	298.2	301.6	298.2	303.2	303.2	303.2	303.2	303.2
Pressure bar	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.1
Vapor Frac	0.0	1.0	1.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0
Liquid Frac	1.0	0.0	0.0	1.0	1.0	0.0	1.0	0.0	0.0	1.0
Solids										
Mass Flow kg/hr										
YEAST	0.0	0.0	0.0	0.0	0.0	0.0	0.4	0.0	0.0	120.0
Total Flow kmol/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.2
Total Flow kg/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.4	0.0	0.0	120.0
Total Flow l/min	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3
Temperature K							303.2			303.2
Pressure bar	1.0	1.0	1.0		1.0	1.0	1.0	1.0	1.0	1.1

1.3 FERMENTATION



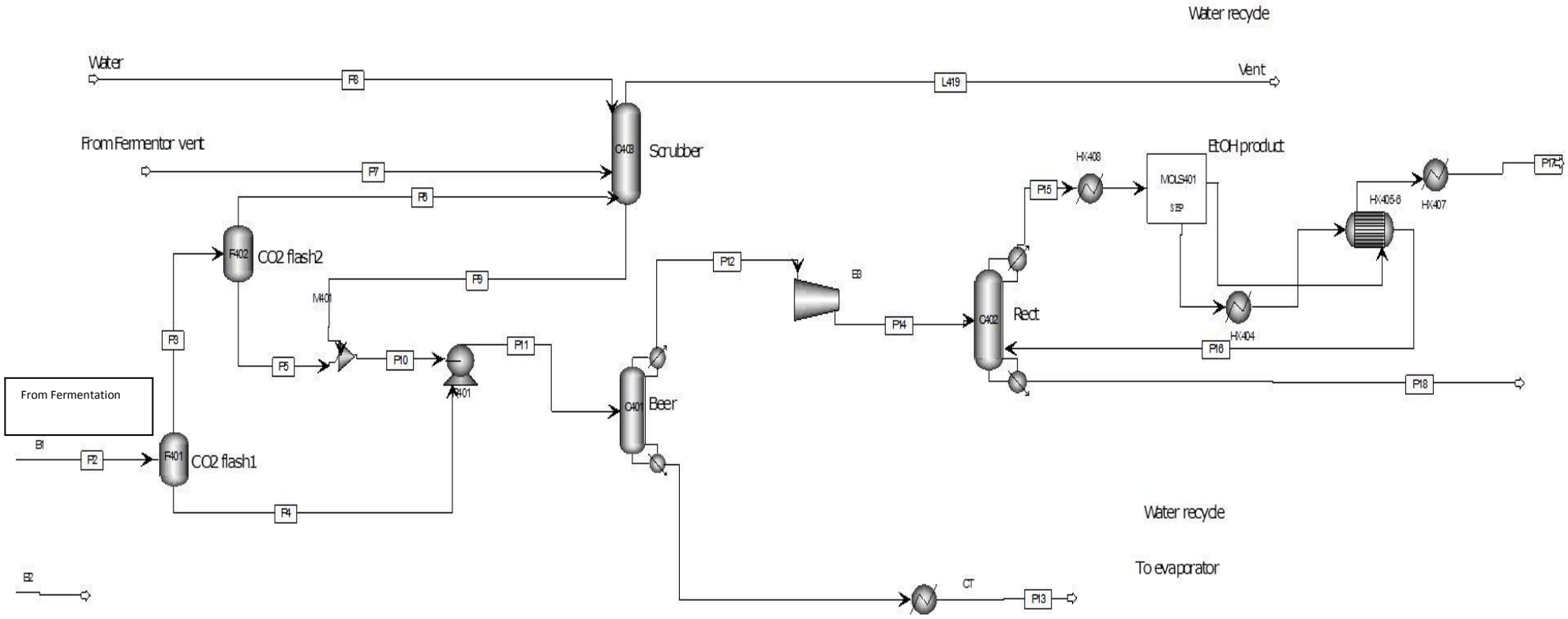
	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10	F11	F12	F13
Substream: MIXED													
Mass Flow kg/hr													
GLUCOSE	0.0	0.0	3614.0	3614.0	0.0	1293.8	1293.8	2320.2	0.0	2320.2	2320.2	0.0	326.5
XYLOSE	0.0	0.0	12625.7	12625.7	0.0	4520.0	4520.0	8105.7	0.0	8105.7	8105.7	0.0	1927.1
ARABINOS	0.0	7.4	931.9	931.9	0.0	333.6	333.6	598.3	0.0	598.3	598.3	0.0	93.9
GALACTOS	0.0	3.0	376.8	376.8	0.0	134.9	134.9	241.9	0.0	241.9	241.9	0.0	36.1
MANNOSE	0.0	0.7	83.7	83.7	0.0	30.0	30.0	53.8	0.0	53.8	53.8	0.0	84.4
CELLOB	0.0	1.1	141.5	141.5	0.0	50.7	50.7	90.9	0.0	90.9	90.9	0.0	0.0
XYLITOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	263.5
EXTRACT	85.7	0.0	3699.8	3699.8	0.0	1324.5	1324.5	2375.3	0.0	2375.3	2375.3	0.0	0.0
ETHANOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	127.6	7514.1
H2O	0.0	540.7	63139.6	63139.6	35983.0	22604.0	58587.0	40535.6	4783.5	35752.1	35752.1	117.1	94761.3
N2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	7142.5	165.8
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	27.7	0.0
NH3	25.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	0.0	6.0	786.8	786.8	0.0	281.7	281.7	505.2	35.9	469.3	469.3	0.5	756.5
NH4SO4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLYCEROL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURF	0.0	2.2	273.9	273.9	0.0	98.1	98.1	175.9	2.6	173.3	173.3	0.0	273.5
Total Flow kmol/hr	1.9	30.2	3653.5	3653.5	1997.4	1308.0	3305.3	2345.5	266.1	2079.4	2079.4	172.4	5460.0
Total Flow kg/hr	110.7	561.2	85673.8	85673.8	35983.0	30671.2	66654.2	55002.6	4821.9	50180.6	50180.6	7415.5	106203.0
Total Flow l/min	572.3	9.3	1281.3	1309.9	601.4	468.9	1075.5	841.0	571657.0	767.6	767.6	64647.9	1792.8
Temperature K	298.2	303.2	301.6	303.3	298.2	303.3	314.2	303.3	324.4	325.3	325.3	303.3	303.3
Pressure bar	1.0	1.1	1.0	1.2	1.0	1.2	1.0	1.2	0.1	0.1	1.0	1.1	1.1
Vapor Frac	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.6	0.0	0.0	1.0	0.0
Liquid Frac	0.3	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.4	1.0	1.0	0.0	1.0
Solids													
Mass Flow kg/hr													
YEAST	0.0	120.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	210.5
Total Flow kmol/hr	0.0	5.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.8
Total Flow kg/hr	0.0	120.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	210.5
Total Flow l/min	0.0	1.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.3
Temperature K		303.2											303.3
Pressure bar	1.0	1.1		1.2	1.0	1.2	1.0	1.2	0.1	0.1	1.0	1.1	1.1

1.4 CONVENTIONAL DISTILLATION

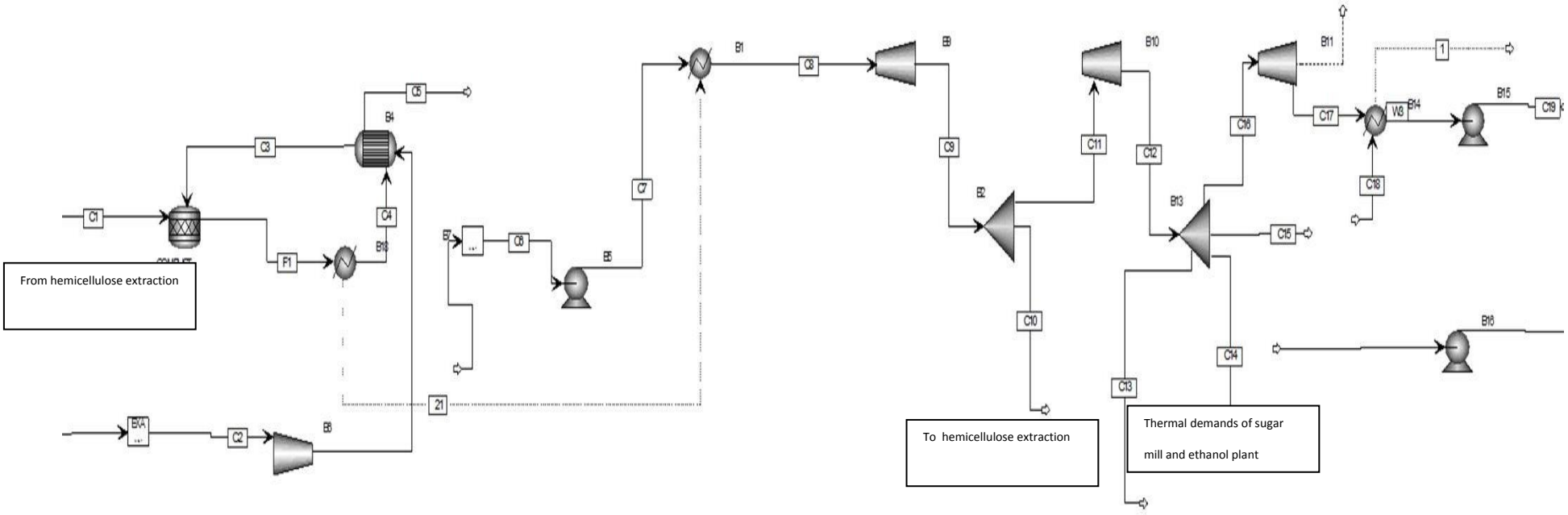


	R 1	R 2	R 3	R 4	R 5	R 6	R 7	R 8	R 9	R 10	R 11	R 12	R 13	R 14	R 15	R 16	R 17
Substream: MIXED																	
Mass Flow kg/hr																	
GLUCOSE	326.5	0.0	326.5	0.0	0.0	0.0	0.0	0.0	326.5	0.0	0.0	326.5	326.5	0.0	0.0	0.0	0.0
XYLOSE	1927.1	0.0	1927.1	0.0	0.0	0.0	0.0	0.0	1927.1	0.0	0.0	1927.1	1927.1	0.0	0.0	0.0	0.0
ACETATE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARABINOS	93.9	0.0	93.9	0.0	0.0	0.0	0.0	0.0	93.9	0.0	0.0	93.9	93.9	0.0	0.0	0.0	0.0
GALACTOS	36.1	0.0	36.1	0.0	0.0	0.0	0.0	0.0	36.1	0.0	0.0	36.1	36.1	0.0	0.0	0.0	0.0
MANNOSE	84.4	0.0	84.4	0.0	0.0	0.0	0.0	0.0	84.4	0.0	0.0	84.4	84.4	0.0	0.0	0.0	0.0
XYLITOL	263.5	0.0	263.5	0.0	0.0	0.0	0.0	0.0	263.5	0.0	0.0	263.5	263.5	0.0	0.0	0.0	0.0
EXTRACT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PROTEIN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ETHANOL	7514.1	181.3	7332.8	168.7	12.7	0.0	127.6	140.1	7641.6	0.2	7618.7	22.9	22.9	9516.7	1903.3	7613.3	5.4
H2O	94761.3	224.8	94536.5	221.0	3.8	10809.5	117.1	10882.4	105640.0	48.1	10788.5	94851.3	94851.3	929.3	924.6	4.6	10783.9
N2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	165.8	155.9	9.9	1.3	154.6	0.0	7142.5	18.0	29.2	7279.1	29.2	0.0	0.0	29.2	0.0	29.2	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	27.7	0.0	0.0	27.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	756.5	0.9	755.6	0.9	0.0	0.0	0.5	0.5	757.0	0.0	38.3	718.6	718.6	0.0	0.0	0.0	38.3
FURFURAL	273.5	0.1	273.4	0.1	0.0	0.0	0.0	0.0	273.5	0.0	3.4	270.2	270.2	0.0	0.0	0.0	3.4
Total Flow kmol/hr	5460.0	20.0	5440.1	16.0	4.0	600.0	172.4	607.5	6063.6	168.9	765.6	5298.0	5298.0	258.8	92.6	166.2	599.4
Total Flow kg/hr	106203.0	563.0	105640.0	391.9	171.1	10809.5	7415.5	11041.1	117073.0	7355.1	18478.2	98594.5	98594.5	10475.1	2828.0	7647.2	10831.0
Total Flow l/min	6514.7	11732.5	1892.2	7.3	1547.6	180.2	64647.9	185.0	2030.6	64637.7	259323.0	1802.1	1636.9	93513.8	60.0	162.6	200.2
Temperature K	359.2	356.5	356.5	311.2	311.2	286.2	303.3	295.2	352.1	287.2	379.2	388.3	308.2	359.5	353.2	298.2	387.5
Pressure bar	1.1	0.8	0.8	1.1	1.1	2.1	1.1	1.0	1.7	1.0	1.6	1.7	1.0	1.4	1.5	1.3	1.7
Vapor Frac	0.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0
Liquid Frac	1.0	0.0	1.0	1.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	1.0	1.0	0.0	1.0	1.0	1.0
Substream: CISOLID																	
Mass Flow kg/hr																	
YEAST	210.5	0.0	210.5	0.0	0.0	0.0	0.0	0.0	210.5	0.0	0.0	210.5	210.5	0.0	0.0	0.0	0.0
Total Flow kmol/hr	8.8	0.0	8.8	0.0	0.0	0.0	0.0	0.0	8.8	0.0	0.0	8.8	8.8	0.0	0.0	0.0	0.0
Total Flow kg/hr	210.5	0.0	210.5	0.0	0.0	0.0	0.0	0.0	210.5	0.0	0.0	210.5	210.5	0.0	0.0	0.0	0.0
Total Flow l/min	2.3	0.0	2.3	0.0	0.0	0.0	0.0	0.0	2.3	0.0	0.0	2.3	2.3	0.0	0.0	0.0	0.0
Temperature K	359.2		356.5						352.1			388.3	308.2				
Pressure bar	1.1	0.8	0.8	1.1	1.1	2.1	1.1	1.0	1.7			1.7	1.0		1.5	1.3	1.7

1.5 VACUUM DISTILLATION

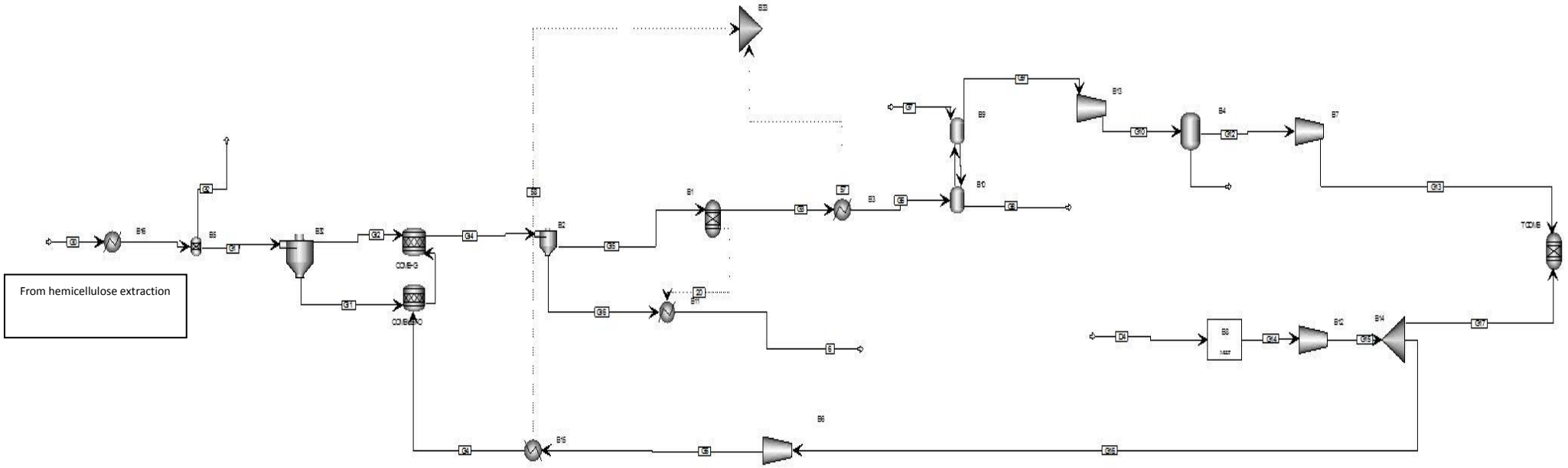


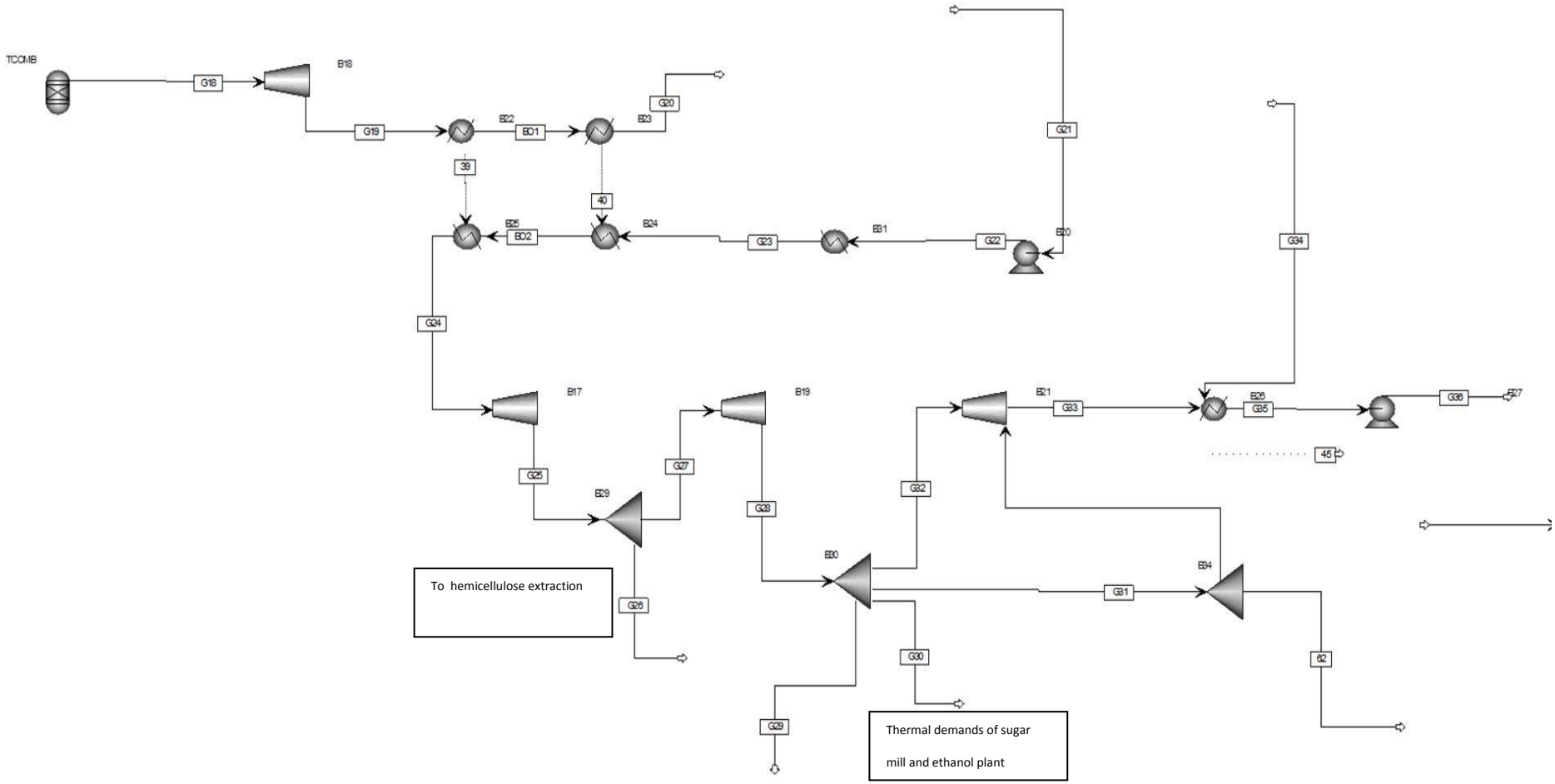
1.6 ENERGY GENERATION COMBUSTION OF PRE-TREATMENT RESIDUES WITH HIGH PRESSURE STEAM CYCLES (CHPSC-CPE)



	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	C19	F1
Substream: MIXED																				
Mass Flow kg/hr																				
GLUCOSE	905.3	0.0	0.0	9.1	9.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	9.1
XYLOSE	3162.6	0.0	0.0	31.6	31.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	31.6
ARABINOS	233.4	0.0	0.0	2.3	2.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.3
GALACTOS	94.4	0.0	0.0	0.9	0.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.9
MANNOSE	21.0	0.0	0.0	0.2	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2
CELLOB	35.5	0.0	0.0	0.4	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.4
EXTRACT	926.8	0.0	0.0	926.8	926.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	926.8
ETHANOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	34573.8	0.0	0.0	61169.7	61169.7	207686.0	207686.0	207686.0	207686.0	16205.3	191481.0	191481.0	27925.1	6425.1	120000.0	37130.8	37130.8	4783.5	41914.3	61169.7
N2	0.0	241799.0	241799.0	241799.0	241799.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	241799.0
CO2	0.0	4489.6	4489.6	90436.6	90436.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	90436.6
O2	0.0	74399.8	74399.8	4093.5	4093.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4093.5
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
AACID	197.1	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	35.9	35.9	2.0
SO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARGON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURF	68.6	0.0	0.0	0.7	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.6	2.6	0.7
H2SO4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	1956.4	11058.6	11058.6	14214.9	14214.9	11528.3	11528.3	11528.3	11528.3	899.5	10628.8	10628.8	1550.1	356.6	6661.0	2061.1	2061.1	266.1	2327.2	14214.9
Total Flow kg/hr	40218.5	320689.0	320689.0	398473.0	398473.0	207686.0	207686.0	207686.0	207686.0	16205.3	191481.0	191481.0	27925.1	6425.1	120000.0	37130.8	37130.8	4821.9	41952.7	398473.0
Total Flow l/min	680.9	4506930.0	7759070.0	11689500.0	8557710.0	3471.3	3570.9	135053.0	469267.0	36567.8	432083.0	1528380.0	223130.0	51338.8	958838.0	296687.0	4212420.0	571657.0	708.0	37121400.0
Temperature K	366.1	298.2	523.2	573.2	420.0	298.2	322.4	787.2	585.2	581.3	581.3	425.5	424.1	424.1	424.1	424.1	333.5	324.4	324.4	1819.3
Pressure bar	1.0	1.0	1.0	1.0	1.0	1.0	86.0	86.0	19.0	19.0	19.0	4.0	4.0	4.0	4.0	4.0	0.2	0.1	1.0	1.0
Vapor Frac	0.0	1.0	1.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.9	0.6	0.0	1.0
Liquid Frac	1.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.4	1.0	0.0
Solids																				
Mass Flow kg/hr																				
CELLULOS	22465.2	0.0	0.0	224.7	224.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	224.7
XYLOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARABINAN	297.9	0.0	0.0	3.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0
MANNAN	38.2	0.0	0.0	0.4	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.4
GALACTAN	171.8	0.0	0.0	1.7	1.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7
ASH	2304.9	0.0	0.0	2304.9	2304.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2304.9
Total Flow kmol/hr	304.9	0.0	0.0	43.7	43.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	43.7
Total Flow kg/hr	40218.5	0.0	0.0	2684.1	2684.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2684.1
Total Flow l/min	513.1	0.0	0.0	16.8	16.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	20.3
Temperature K	366.1			573.2	420.0															1819.3
Pressure bar	1.0	1.0	1.0	1.0	1.0	1.0	86.0	86.0	19.0	19.0	19.0	4.0	4.0	4.0	4.0	4.0	0.2	0.1	1.0	1.0

1.7 ENERGY GENERATION FROM PRE-TREATMENT RESIDUES WITH BIOMASS INTEGRATED GASIFICATION AND COMBINED CYCLES (BIGCC-CPE)

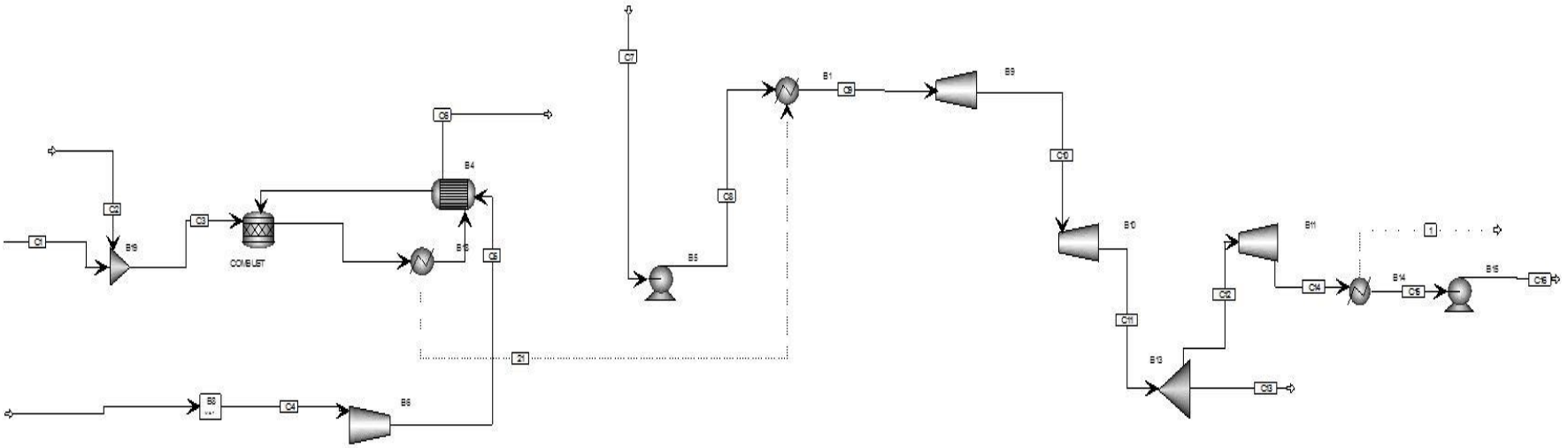




	GI1	GI2	GI3	GI4	GI5	GI6	G0	G1	G2	G3	G4	G5	G6	G8	G9	G10	G11	G12	G13	G14
Substream: MIXED																				
Mass Flow kg/hr																				
GLUCOSE	0.0	911.6	0.0	0.0	0.0	0.0	911.6	911.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLOSE	0.0	3184.8	0.0	0.0	0.0	0.0	3184.8	3184.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETATE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARABINOSE	0.0	235.1	0.0	0.0	0.0	0.0	235.1	235.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GALACTOSE	0.0	95.0	0.0	0.0	0.0	0.0	95.0	95.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MANNOSE	0.0	21.1	0.0	0.0	0.0	0.0	21.1	21.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLITOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
EXTRACT	0.0	0.0	0.0	0.0	0.0	0.0	933.3	0.0	933.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ETHANOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	0.0	7097.4	1649.7	11583.4	11583.4	0.0	34534.3	7097.4	27436.9	11729.0	0.0	0.0	11729.0	95271.7	16457.3	16457.3	11708.7	4748.6	4748.6	0.0
N2	0.0	0.0	91721.8	91721.8	91721.8	0.0	0.0	0.0	0.0	91721.8	91721.8	91721.8	91721.8	0.6	91721.2	91721.2	0.7	91720.5	91720.5	584374.0
CO2	0.0	0.0	32504.2	25479.9	25479.9	0.0	0.0	0.0	0.0	25126.1	1703.1	1703.1	25126.1	6.3	25119.8	25119.8	5.6	25114.2	25114.2	10850.4
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	28222.1	28222.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	179807.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	0.0	198.5	0.0	2.0	2.0	0.0	198.5	198.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLYCEROL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NUTRIENT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	31174.7	40116.0	40116.0	0.0	0.0	0.0	0.0	40342.3	0.0	0.0	40342.3	0.4	40341.9	40341.9	0.4	40341.5	40341.5	0.0
ARGON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURAL	0.0	69.1	0.0	0.7	0.7	0.0	69.1	69.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2SO4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HMF	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	2504.1	2504.1	2504.1	0.0	0.0	0.0	0.0	2487.8	0.0	0.0	2487.8	0.0	2487.8	2487.8	0.0	2487.8	2487.8	0.0
Total Flow kmol/hr	0.0	426.7	6459.5	7170.6	7170.6	0.0	1954.5	426.7	1527.8	7170.6	4194.9	4194.9	7170.6	5288.6	7432.9	7432.9	650.1	6782.8	6782.8	26726.2
Total Flow kg/hr	0.0	11848.3	159555.0	171408.0	171408.0	0.0	40218.5	11848.3	28370.2	171408.0	121647.0	121647.0	171408.0	95279.0	176129.0	176129.0	11715.5	164414.0	164414.0	775032.0
Total Flow l/min	0.0	186.7	12531300.0	11470900.0	11470900.0	0.0	680.6	186.7	468.5	11461100.0	6328680.0	2258750.0	3638500.0	1607.1	3282010.0	672838.0	200.3	325603.0	205652.0	10891400.0
Temperature K		341.2	1418.2	1169.5	1169.5		366.2	341.2	341.2	1168.5	1103.2	393.7	371.2	322.9	323.2	653.2	347.2	347.2	436.2	298.2
Pressure bar		1.0	1.0	1.0	1.0		1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	10.0	10.0	10.0	20.0	1.0
Vapor Frac		0.0	1.0	1.0	1.0		0.0	0.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0	1.0
Liquid Frac		1.0	0.0	0.0	0.0		1.0	1.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0
Substream: CISOLID																				
Mass Flow kg/hr																				
CELLULOS	22465.2	0.0	0.0	0.0	0.0	0.0	22465.2	22465.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLAN	403.6	0.0	0.0	0.0	0.0	0.0	403.6	403.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LIGNIN	14536.9	0.0	0.0	0.0	0.0	0.0	14536.9	14536.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARABINAN	297.9	0.0	3.0	0.0	0.0	0.0	297.9	297.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MANNAN	38.2	0.0	0.4	0.0	0.0	0.0	38.2	38.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GALACTAN	171.8	0.0	1.7	0.0	0.0	0.0	171.8	171.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PROTEIN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH	2304.9	0.0	2304.9	2304.9	0.0	2304.9	2304.9	2304.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	304.9	0.0	41.1	41.1	0.0	41.1	304.9	304.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	40218.5	0.0	2310.0	2305.0	0.0	2305.0	40218.5	40218.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow l/min	510.0	0.0	11.6	11.5	0.0	11.5	513.1	510.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Temperature K	341.2		1418.2	1169.5		1169.5	366.2	341.2												
Pressure bar	1.0		1.0	1.0		1.0	1.0	1.0	1.0			1.0	1.0	1.0	1.0	10.0	10.0	10.0	20.0	1.0

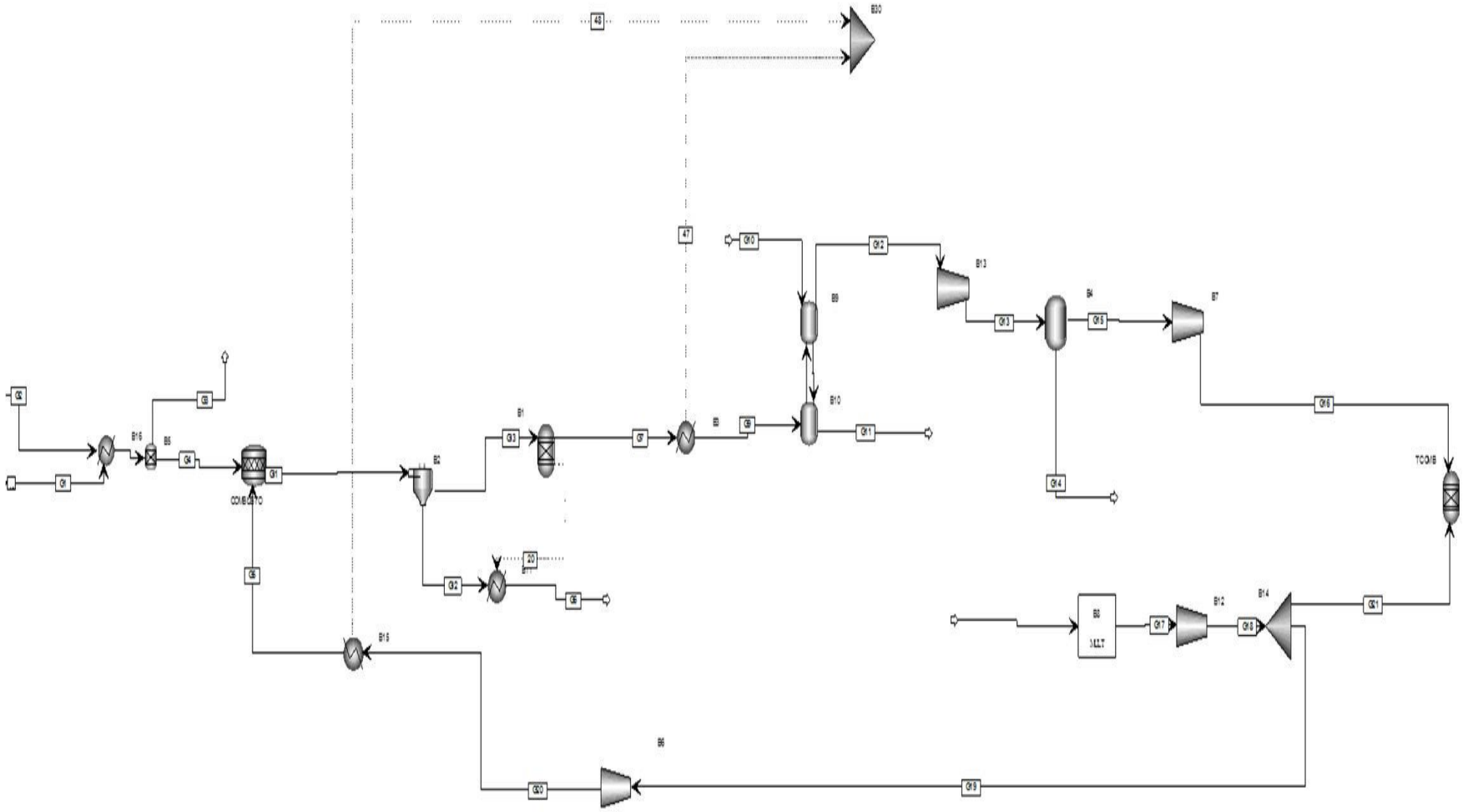
	G15	G16	G17	G18	G19	G20	G21	G22	G23	G24	G25	G26	G27	G28	G29	G30	G31	G32	G33	G34	G35	G36
Substream: MIXED																						
Mass Flow kg/hr																						
GLUCOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETATE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARABINOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GALACTOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MANNOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLITOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
EXTRACT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ETHANOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	0.0	0.0	0.0	26983.1	26983.1	26983.1	149181.0	149181.0	149181.0	149181.0	149181.0	16705.3	132475.0	132475.0	6425.1	120000.0	5407.6	642.6	1542.6	4724.8	6267.4	6267.4
N2	584374.0	91721.8	492652.0	584168.0	584168.0	584168.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	10850.4	1703.1	9147.4	97648.7	97648.7	97648.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	179807.0	28222.1	151585.0	108555.0	108555.0	108555.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	429.7	429.7	429.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	0.0	14.5	14.5	14.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	35.5	35.5	35.5
GLYCEROL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NUTRIENT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARGON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	2.5	2.5
H2SO4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HMF	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	26726.2	4194.9	22531.3	27976.8	27976.8	27976.8	8280.8	8280.8	8280.8	8280.8	8280.8	927.3	7353.5	7353.5	356.6	6661.0	300.2	35.7	85.6	262.9	348.5	348.5
Total Flow kg/hr	775032.0	121647.0	653385.0	817798.0	817798.0	817798.0	149181.0	149181.0	149181.0	149181.0	149181.0	16705.3	132475.0	132475.0	6425.1	120000.0	5407.6	642.6	1542.6	4762.9	6305.5	6305.5
Total Flow l/min	1666360.0	261548.0	1404810.0	3348690.0	30068900.0	18103200.0	2493.4	2487.3	13442.8	128695.0	331255.0	37094.0	294161.0	1040470.0	50463.2	942486.0	42471.7	5047.0	176180.0	565531.0	106.4	106.4
Temperature K	716.3	716.3	716.3	1377.6	785.7	473.2	298.2	298.8	548.7	723.2	573.0	573.0	573.0	417.3	417.3	417.3	417.3	417.3	333.2	324.4	324.4	324.5
Pressure bar	16.0	16.0	16.0	16.0	1.0	1.0	1.0	60.0	60.0	60.0	19.0	19.0	19.0	4.0	4.0	4.0	4.0	4.0	0.2	0.1	0.1	1.0
Vapor Frac	1.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	0.1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.9	0.6	0.0	0.0
Liquid Frac	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.4	1.0	1.0
Substream: CISOLID																						
Mass Flow kg/hr																						
CELLULOS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLAN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LIGNIN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARABINAN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MANNAN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GALACTAN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PROTEIN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow l/min	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Temperature K																						
Pressure bar	16.0	16.0	16.0		1.0	1.0	1.0	60.0	60.0	60.0	19.0	19.0	19.0	4.0	4.0	4.0	4.0	4.0	0.2	0.1	0.1	1.0

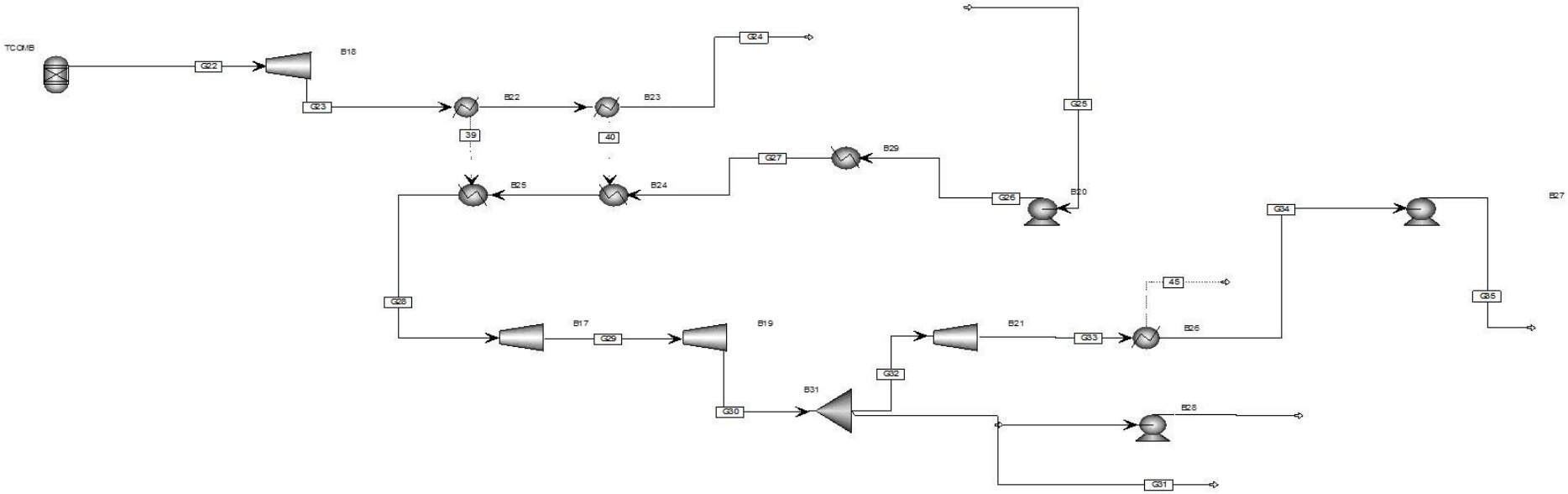
1.8 EXCLUSIVE ELECTRICITY PRODUCTION FROM BIOMASS COMBUSTION HIGH PRESSURE STEAM CYCLES (CHPSC-EE)



	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16
Substream: MIXED																
EXTRACT	3150.0	1506.1	4656.1	0.0	0.0	4656.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	42000.0	4000.6	46000.6	0.0	0.0	81337.3	277221.0	277221.0	277221.0	277221.0	277221.0	157221.0	120000.0	157221.0	157221.0	157221.0
N2	0.0	0.0	0.0	311716.0	311716.0	311716.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	5787.8	5787.8	119717.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	95912.6	95912.6	5261.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	2347.6	229.8	2577.4	14256.2	14256.2	18550.9	15388.1	15388.1	15388.1	15388.1	15388.1	8727.1	6661.0	8727.1	8727.1	8727.1
Total Flow kg/hr	45150.0	5506.7	50656.7	413416.0	413416.0	522687.0	277221.0	277221.0	277221.0	277221.0	277221.0	157221.0	120000.0	157221.0	157221.0	157221.0
Total Flow l/min	706.5	69.0	775.2	5810110.0	5733630.0	11082900.0	4633.5	4766.2	180513.0	856754.0	2219460.0	1260030.0	961728.0	17852700.0	2665.7	2665.6
Temperature K	298.2	298.2	296.9	298.2	300.1	423.0	298.2	322.4	788.0	543.8	426.7	425.3	425.3	333.5	333.5	333.5
Pressure bar	1.0	1.0	1.0	1.0	1.0	1.0	1.0	86.0	86.0	13.0	4.0	4.0	4.0	0.2	0.2	1.0
Vapor Frac	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0	0.9	0.0	0.0
Liquid Frac	1.0	1.0	1.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.1	1.0	1.0
Solids																
Mass Flow kg/hr																
CELLULOS	17052.0	9666.8	26718.8	0.0	0.0	267.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLAN	9702.0	6187.1	15889.1	0.0	0.0	158.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LIGNIN	9072.0	5464.9	14536.9	0.0	0.0	145.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARABINAN	840.0	490.0	1330.0	0.0	0.0	13.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MANNAN	84.0	49.0	133.0	0.0	0.0	1.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GALACTAN	378.0	220.5	598.5	0.0	0.0	6.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH	1722.0	582.9	2304.9	0.0	0.0	2304.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	292.6	166.8	459.4	0.0	0.0	45.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	38850.0	22661.2	61511.2	0.0	0.0	2897.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow l/min	474.8	278.5	753.1	0.0	0.0	19.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Temperature K	298.2	298.2	296.9			423.0										
Pressure bar	1.0	1.0	1.0	1.0	1.0	1.0	1.0	86.0	86.0	13.0	4.0	4.0	4.0	0.2	0.2	1.0

1.9 ENERGY GENERATION FROM PRE-TREATMENT RESIDUES WITH BIOMASS INTEGRATED GASIFICATION AND COMBINED CYCLES (BIGCC-CPE)





	GI1	GI2	GI3	G1	G2	G3	G4	G5	G6	G7	G9	G10	G11	G12	G13	G14
Substream: MIXED																
Mole Flow kmol/hr																
Mass Flow kg/hr																
EXTRACT	0.0	0.0	0.0	3150.0	1506.1	4656.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ETHANOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	20667.2	0.0	20667.2	42000.0	4000.6	35145.7	10854.9	0.0	0.0	16331.5	16331.5	100000.0	95388.4	20943.1	20943.1	10806.1
N2	110916.0	0.0	110916.0	0.0	0.0	0.0	0.0	110916.0	0.0	110916.0	110916.0	0.0	0.6	110916.0	110916.0	0.4
CO2	22372.4	0.0	22372.4	0.0	0.0	0.0	0.0	2059.4	0.0	32967.4	32967.4	0.0	6.3	32961.1	32961.1	3.2
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	34128.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.2	1.2	0.0	0.0	1.2	1.2	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	60292.9	0.0	60292.9	0.0	0.0	0.0	0.0	0.0	0.0	53547.6	53547.6	0.0	0.4	53547.2	53547.2	0.3
HYDROGEN	2894.8	0.0	2894.8	0.0	0.0	0.0	0.0	0.0	0.0	3379.6	3379.6	0.0	0.0	3379.6	3379.6	0.0
Total Flow kmol/hr	9203.4	0.0	9203.4	2347.6	229.8	1974.9	602.5	5072.7	0.0	9203.3	9203.3	5550.8	5295.0	9459.1	9459.1	599.9
Total Flow kg/hr	217143.0	0.0	217143.0	45150.0	5506.7	39801.8	10854.9	147104.0	0.0	217143.0	217143.0	100000.0	95395.7	221748.0	221748.0	10809.9
Total Flow l/min	14566100.0	0.0	14566100.0	706.5	69.0	605.3	184.8	7653050.0	0.0	14868700.0	4669820.0	1671.4	1609.8	4176750.0	1230760.0	184.8
Temperature K	1157.0		1157.0	298.2	298.2	341.2	341.2	1103.2		1181.1	371.2	298.2	323.8	323.2	563.4	347.2
Pressure bar	1.0		1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	6.0	6.0
Vapor Frac	1.0		1.0	0.0	0.0	0.0	0.0	1.0		1.0	1.0	0.0	0.0	1.0	1.0	0.0
Liquid Frac	0.0		0.0	1.0	1.0	1.0	1.0	0.0		0.0	0.0	1.0	1.0	0.0	0.0	1.0
Solid Frac	0.0		0.0	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0
Substream: CISOLID																
Mass Flow kg/hr																
CELLULOSE	0.0	0.0	0.0	17052.0	9666.8	0.0	26718.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLAN	0.0	0.0	0.0	9702.0	6187.1	0.0	15889.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LIGNIN	0.0	0.0	0.0	9072.0	5464.9	0.0	14536.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARABINAN	13.3	13.3	0.0	840.0	490.0	0.0	1330.0	0.0	13.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MANNAN	1.3	1.3	0.0	84.0	49.0	0.0	133.0	0.0	1.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GALACTAN	6.0	6.0	0.0	378.0	220.5	0.0	598.5	0.0	6.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PROTEIN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH	2304.9	2304.9	0.0	1722.0	582.9	0.0	2304.9	0.0	2304.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	41.2	41.2	0.0	292.6	166.8	0.0	459.4	0.0	41.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	2325.5	2325.5	0.0	38850.0	22661.2	0.0	61511.2	0.0	2325.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow l/min	11.8	11.8	0.0	474.8	278.5	0.0	759.4	0.0	11.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Temperature K	1157.0	1157.0		298.2	298.2		341.2		1181.1							
Pressure bar	1.0	1.0		1.0	1.0	1.0	1.0	1.0	1.0		1.0	1.0	1.0	1.0	6.0	6.0

	G15	G16	G17	G18	G19	G20	G21	G22	G23	G24	G25	G26	G27	G28	G29	G30	G31	G32	G33	G34	G35
Substream: MIXED																					
Mole Flow kmol/hr																					
Mass Flow kg/hr																					
EXTRACT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ETHANOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	10137.0	10137.0	0.0	0.0	0.0	0.0	0.0	40342.1	40342.1	40342.1	191984.0	191984.0	191984.0	191984.0	191984.0	191984.0	120000.0	71983.7	71983.7	71983.7	71983.7
N2	110915.0	110915.0	784157.0	784157.0	110916.0	110916.0	673241.0	783863.0	783863.0	783863.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	32957.9	32957.9	14559.9	14559.9	2059.4	2059.4	12500.5	129594.0	129594.0	129594.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	241279.0	241279.0	34128.0	34128.0	207151.0	149396.0	149396.0	149396.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	1.2	1.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	615.1	615.1	615.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	20.2	20.2	20.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	53546.9	53546.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HYDROGEN	3379.6	3379.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	8859.2	8859.2	35863.2	35863.2	5072.7	5072.7	30790.5	37855.4	37855.4	37855.4	10656.7	10656.7	10656.7	10656.7	10656.7	10656.7	6661.0	3995.7	3995.7	3995.7	3995.7
Total Flow kg/hr	210938.0	210938.0	1040000.0	1040000.0	147104.0	147104.0	892892.0	1103830.0	1103830.0	1103830.0	191984.0	191984.0	191984.0	191984.0	191984.0	191984.0	120000.0	71983.7	71983.7	71983.7	71983.7
Total Flow l/min	708918.0	312180.0	14616000.0	2222300.0	314336.0	2727390.0	1907960.0	4560810.0	41002100.0	24495200.0	3208.8	3200.9	8289.2	165465.0	575386.0	1506140.0	941420.0	564724.0	8218400.0	1220.3	1220.3
Temperature K	347.2	508.6	298.2	715.5	715.5	393.1	715.5	1386.6	792.0	473.2	298.2	298.7	548.7	722.6	532.6	416.8	416.8	416.8	333.2	333.2	333.2
Pressure bar	6.0	20.0	1.0	16.0	16.0	1.0	16.0	16.0	1.0	1.0	1.0	60.0	60.0	60.0	13.2	4.0	4.0	4.0	0.2	0.2	1.0
Vapor Frac	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0	0.9	0.0	0.0
Liquid Frac	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.1	1.0	1.0
Solid Frac	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Substream: CISOLID																					
Mass Flow kg/hr																					
CELLULOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLAN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LIGNIN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARABINAN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MANNAN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GALACTAN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PROTEIN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow l/min	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Temperature K																					
Pressure bar	6.0	20.0	1.0	16.0	16.0	1.0	16.0		1.0	1.0	1.0	60.0	60.0	60.0	13.2	4.0	4.0	4.0	0.2	0.2	1.0

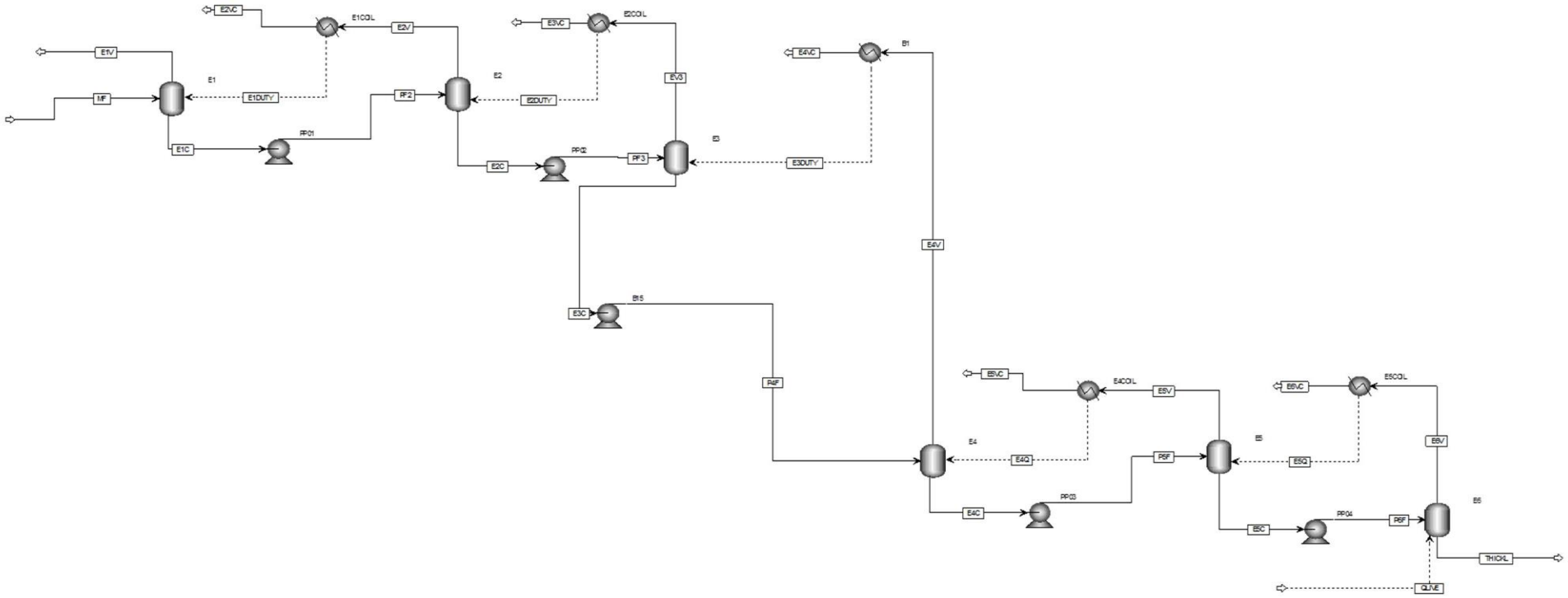
2. APPENDIX D2

Table D 14: Configuration of flow sheets for Chapter 5 (20DS-- Spent sulphite liquor (SSL) substrate concentrated to a dissolved solid concentration of 20%; 30DS-- SSL substrate concentrated to a dissolved solid concentration of 30%; CON – conventional distillation; ME – multi-effect distillation; CS – Energy supply with coal, BD – Energy supplementation with biodigestion of liquid effluent; BB – Energy supply with a biomass-fed boiler)

Overall Scenarios		Subsections/Component flow-sheets												
		6 - Effect Concentration	4 - Effect Concentration	5 - Effect Concentration	Seed Train	Fermentation	Multi-effect Distillation	Conventional Distillation	2-Effect Post Distillation Concentration	1-Effect Post Distillation Concentration	Recovery Boiler	Coal Boilers	Biomass Boilers	Digestion
Flow Sheets	Reference Flow Sheet	X									X			
	20DS-ME-CS		X		X	X	X		X		X	X		
	20DS-CON-CS		X		X	X		X	X		X	X		
	30DS-ME-CS			X	X	X	X			X	X	X		
	30DS-CON-CS*			X	X	X		X		X	X	X		
	20DS-ME-CS-BD		X		X	X	X		X		X	X		X
	20DS-CON-CS-BD		X		X	X		X	X		X	X		X
	30DS-ME-CS-BD			X	X	X	X			X	X	X		X
	30DS-CON-CS-BD*			X	X	X		X		X	X	X		X
	20DS-ME-BB		X		X	X	X		X		X		X	
	20DS-CON-BB		X		X	X		X	X		X		X	
	30DS-ME-BB			X	X	X	X			X	X		X	
	30DS-CON-BB*			X	X	X		X		X	X		X	
	20DS-ME-BB-BD		X		X	X	X		X		X		X	X
	20DS-CON-BB-BD		X		X	X		X	X		X		X	X
	30DS-ME-BB-BD			X	X	X	X			X	X		X	X
	30DS-CON-BB-BD*			X	X	X		X		X	X		X	X

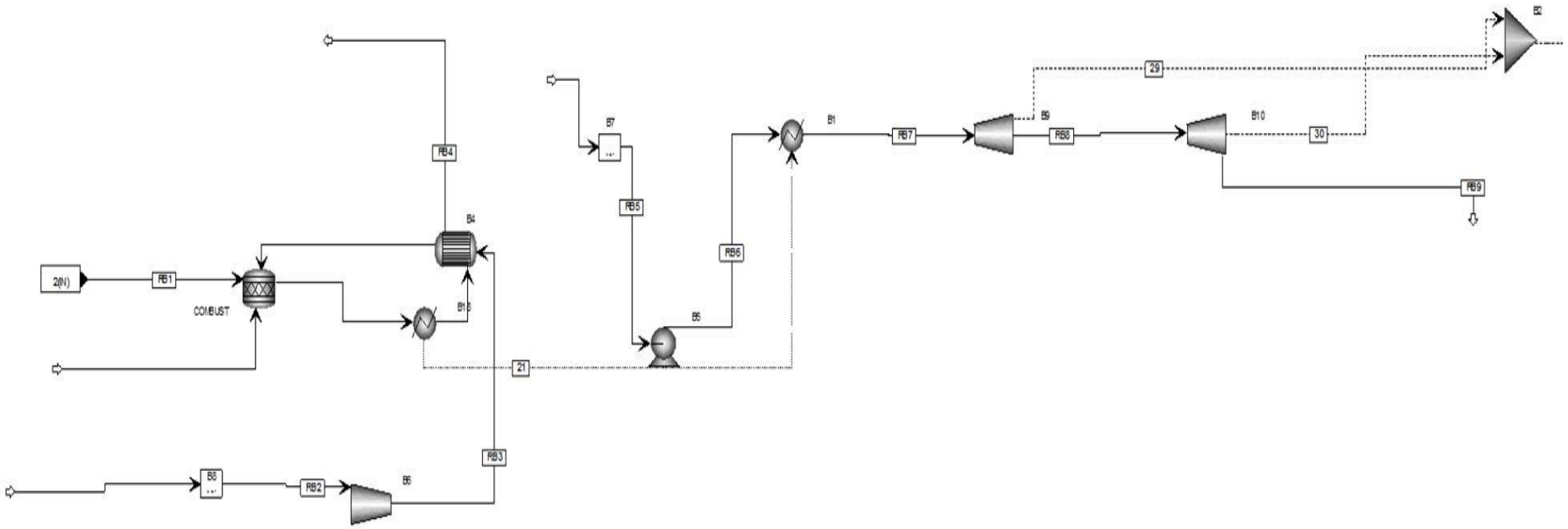
*full mass balance represented

2.1 REFERENCE FLOW SHEET – 6-EFFECT EVAPORATION



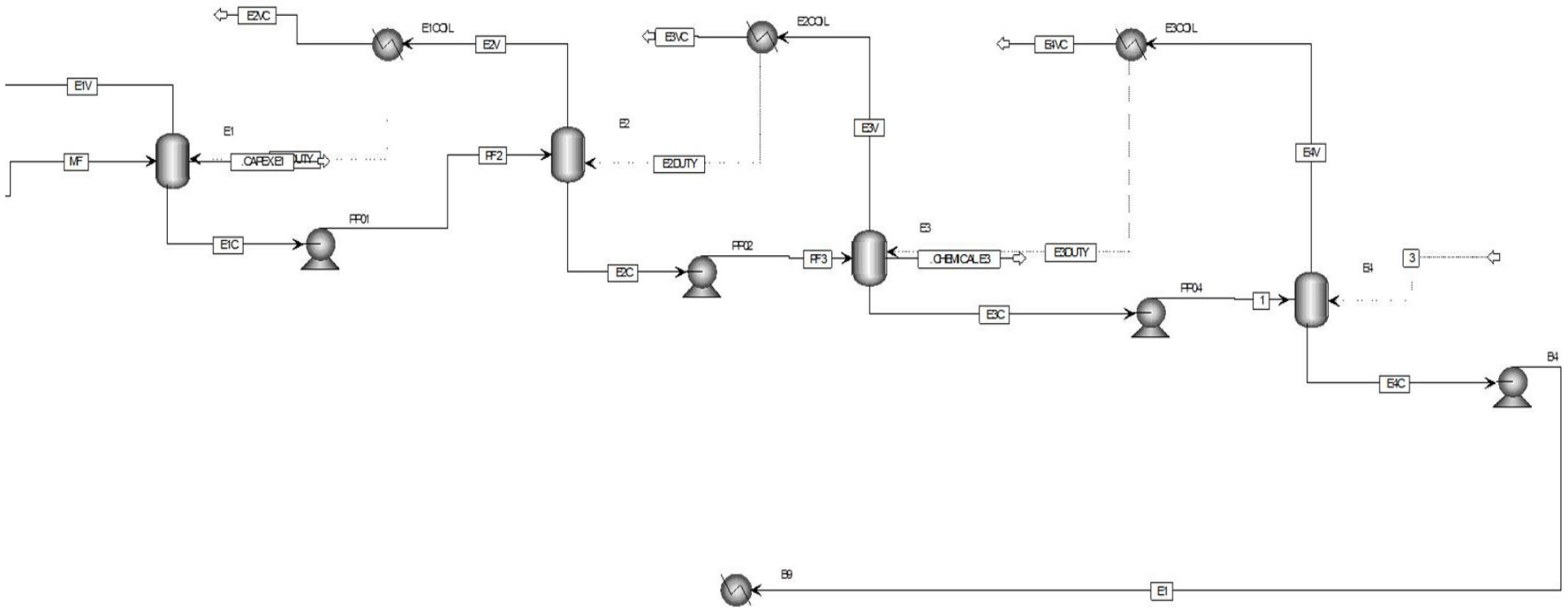
	MF	E1C	E1V	E2C	E2V	E2VC	E3C	EV3	E3VC	E4C	E4V	E4VC	E5C	E5V	E5VC	E6V	E6VC	THICKL
Substream: MIXED																		
Mass Flow kg/hr																		
GLUCOSE	332.8	332.8	0.0	332.8	0.0	0.0	332.8	0.0	0.0	332.8	0.0	0.0	332.8	0.0	0.0	0.0	0.0	332.8
XYLOSE	4249.6	4249.6	0.0	4249.6	0.0	0.0	4249.6	0.0	0.0	4249.6	0.0	0.0	4249.6	0.0	0.0	0.0	0.0	4249.6
ARABINOS	204.8	204.8	0.0	204.8	0.0	0.0	204.8	0.0	0.0	204.8	0.0	0.0	204.8	0.0	0.0	0.0	0.0	204.8
H2O	226712.0	192455.0	34256.9	168372.0	24083.3	24083.3	138687.0	29685.2	29685.2	103709.0	34978.1	34978.1	64187.9	39520.7	39520.7	42094.0	42094.0	22093.9
ACETIC ACID	998.4	904.9	93.5	836.7	68.3	68.3	746.8	89.8	89.8	629.1	117.7	117.7	470.2	158.9	158.9	237.6	237.6	232.6
FURFURAL	51.2	50.2	1.0	49.4	0.8	0.8	48.0	1.3	1.3	45.9	2.1	2.1	42.2	3.7	3.7	9.8	9.8	32.4
FORMIC ACID	179.2	144.6	34.6	123.5	21.1	21.1	100.5	23.0	23.0	75.8	24.7	24.7	48.8	26.9	26.9	29.1	29.1	19.7
MG-O LGSPNT	23270.3	23270.3	0.0	23270.3	0.0	0.0	23270.3	0.0	0.0	23270.3	0.0	0.0	23270.3	0.0	0.0	0.0	0.0	23270.3
Total Flow kmol/hr	13670.4	11766.5	1903.9	10428.1	1338.4	1338.4	8778.3	1649.8	1649.8	6834.2	1944.1	1944.1	4637.2	2197.0	2197.0	2341.3	2341.3	2296.0
Total Flow kg/hr	255999.0	221612.0	34386.0	197439.0	24173.5	24173.5	167640.0	29799.4	29799.4	132517.0	35122.6	35122.6	92806.6	39710.3	39710.3	42370.6	42370.6	50436.0
Total Flow cum/hr	255.0	216.4	365389.0	193.5	137882.0	24.7	164.8	95276.8	30.7	130.1	65575.7	36.6	89.7	52239.6	41.7	35111.3	45.1	46.2
Temperature C	80.0	54.8	54.8	69.7	69.7	67.2	85.3	85.3	82.0	102.1	102.1	97.3	116.2	116.2	108.3	146.7	124.8	146.7
Pressure atm	2.0	0.1	0.1	0.3	0.3	0.3	0.5	0.5	0.5	0.9	0.9	0.9	1.3	1.3	1.3	2.3	2.3	2.3
Vapor Frac	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0
Liquid Frac	1.0	1.0	0.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0	1.0	0.0	1.0	1.0
SOLIDS																		
Mass Flow kg/hr																		
ASH	2912.1	2912.1	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	0.0	0.0	2912.1
Total Flow kmol/hr	51.9	51.9	0.0	51.9	0.0	0.0	51.9	0.0	0.0	51.9	0.0	0.0	51.9	0.0	0.0	0.0	0.0	51.9
Total Flow kg/hr	2912.1	2912.1	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	0.0	0.0	2912.1
Total Flow cum/hr	0.9	0.9	0.0	0.9	0.0	0.0	0.9	0.0	0.0	0.9	0.0	0.0	0.9	0.0	0.0	0.0	0.0	0.9
Temperature C	80.0	54.8		69.7			85.3			102.1			116.2					146.7
Pressure atm	2.0	0.1	0.1	0.3	0.3	0.3	0.5	0.5	0.5	0.9	0.9	0.9	1.3	1.3	1.3	2.3	2.3	2.3

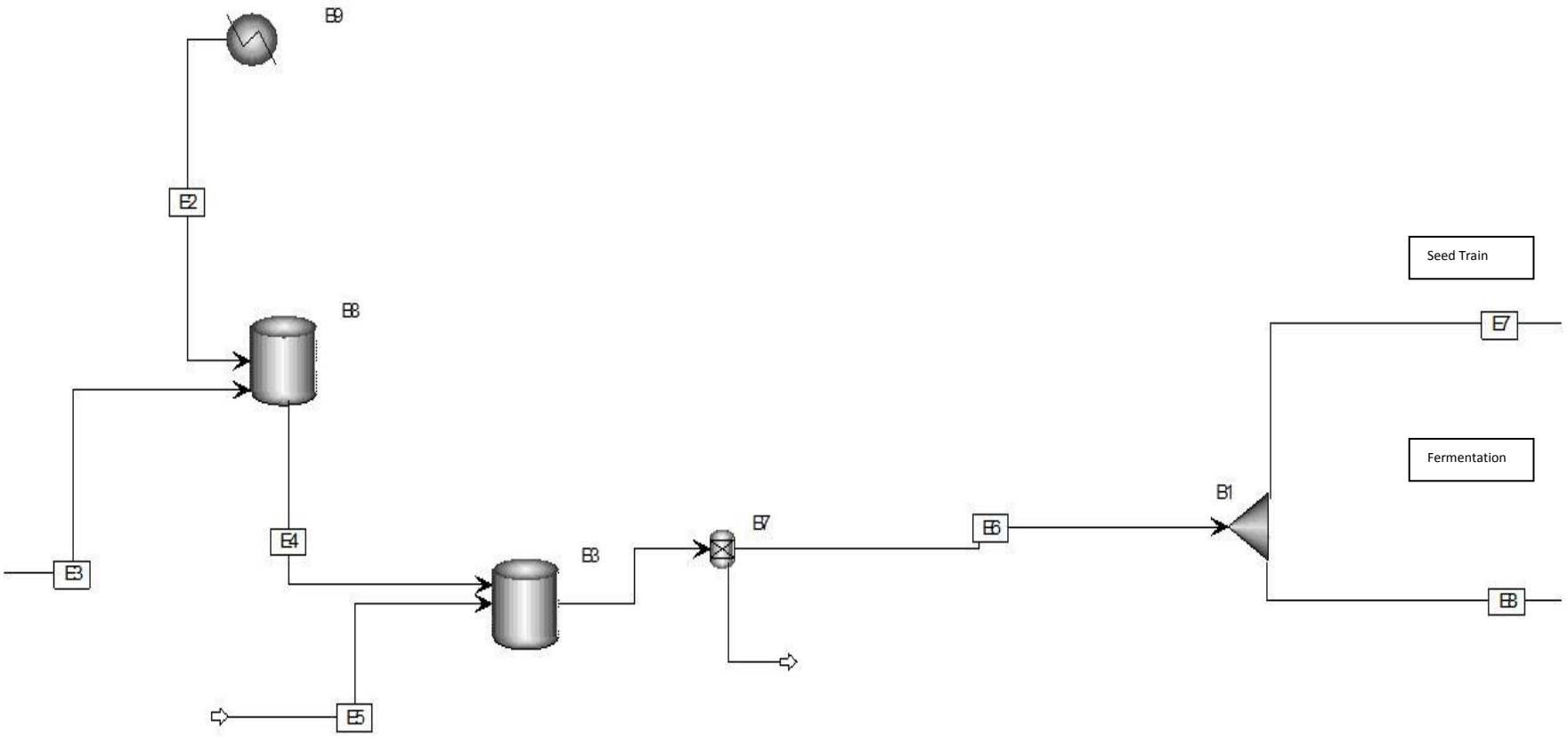
2.2 REFERENCE FLOW SHEET – RECOVERY BOILER



	RB1	RB2	RB3	RB4	RB5	RB6	RB7	RB8	RB9
Substream: MIXED									
Mass Flow kg/hr									
GLUCOSE	332.8	0.0	0.0	3.3	0.0	0.0	0.0	0.0	0.0
XYLOSE	4249.6	0.0	0.0	42.5	0.0	0.0	0.0	0.0	0.0
ARABINOSE	204.8	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0
H2O	22093.9	0.0	0.0	30894.0	136103.0	136103.0	136103.0	136103.0	136103.0
N2	0.0	167716.0	167716.0	169227.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	3114.1	3114.1	55969.9	0.0	0.0	0.0	0.0	0.0
O2	0.0	51604.9	51604.9	9254.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	232.6	0.0	0.0	2.3	0.0	0.0	0.0	0.0	0.0
SO2	0.0	0.0	0.0	7360.4	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURAL	32.4	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.0
H2SO4	0.0	0.0	0.0	113.8	0.0	0.0	0.0	0.0	0.0
HMF									
FORMIC ACID	19.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MG-O LGSPNT	23270.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	2296.0	7670.4	7670.4	9433.2	7554.8	7554.8	7554.8	7554.8	7554.8
Total Flow kg/hr	50436.0	222435.0	222435.0	272870.0	136103.0	136103.0	136103.0	136103.0	136103.0
Total Flow cum/hr	46.2	187565.0	185096.0	311602.0	136.5	140.4	8675.9	15103.4	38068.6
Temperature C	146.7	25.0	27.0	137.8	25.0	49.0	445.0	358.1	227.2
Pressure atm	2.3	1.0	1.0	1.0	1.0	48.4	48.4	24.7	7.9
Vapor Frac	0.0	1.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0
Liquid Frac	1.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
Solid Frac	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Solids									
Mass Flow kg/hr									
ASH	2912.1	0.0	0.0	2912.1	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	51.9	0.0	0.0	51.9	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	2912.1	0.0	0.0	2912.1	0.0	0.0	0.0	0.0	0.0
Total Flow cum/hr	0.9	0.0	0.0	0.9	0.0	0.0	0.0	0.0	0.0
Temperature C	146.7			137.8					
Pressure atm	2.3	1.0	1.0	1.0	1.0	48.4	48.4	24.7	7.9

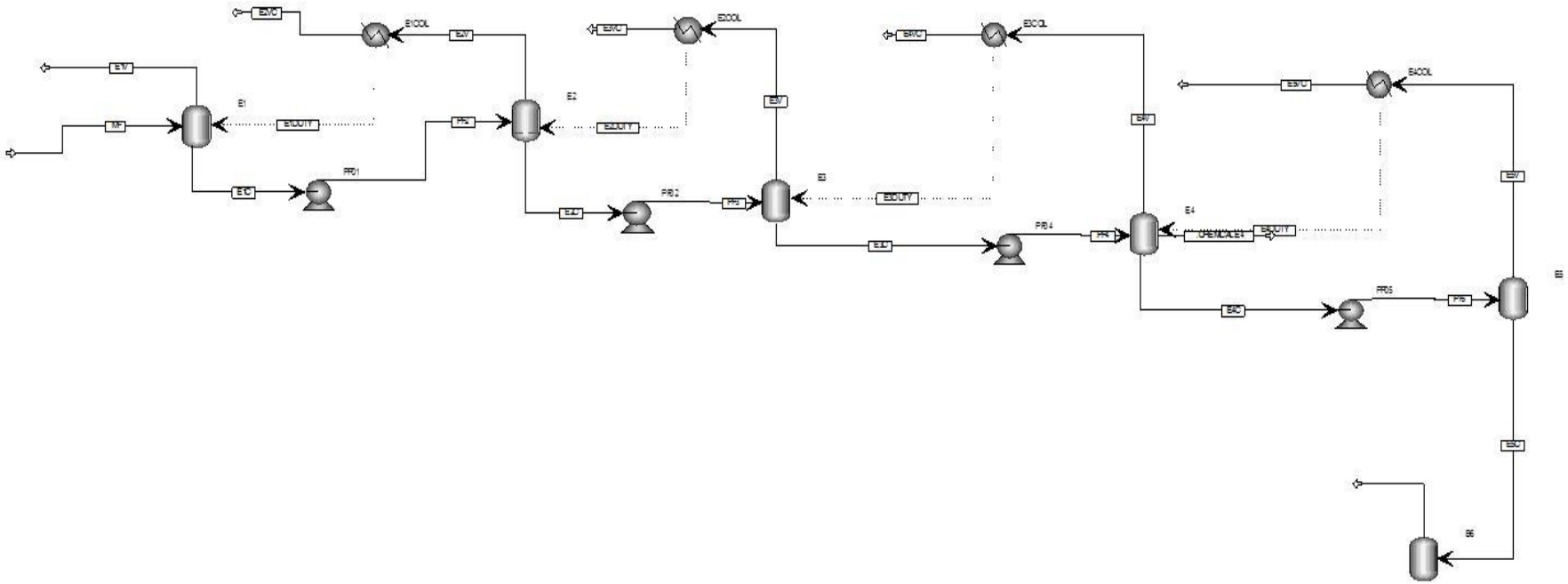
2.3 4 –EFFECT CONCENTRATION AND DETOXIFICATION

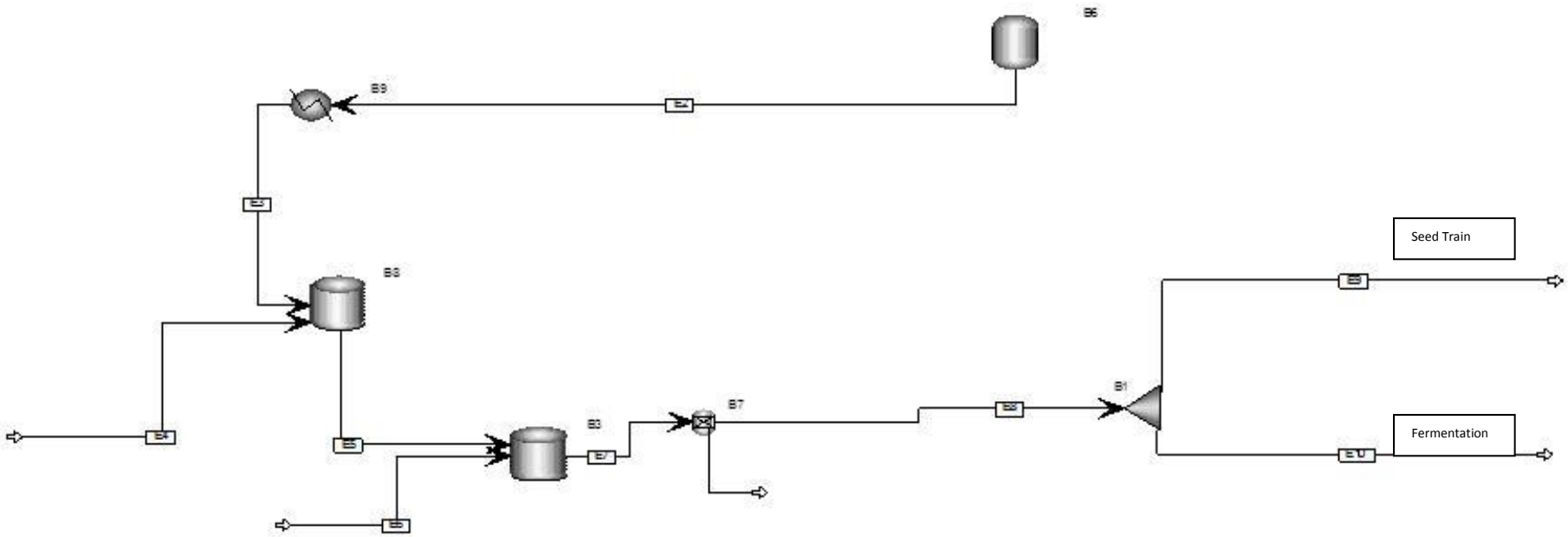




	MF	E1C	E1V	E2C	E2V	E2VC	E3C	E3V	E3VC	E4C	E4V	E4VC	E1	E2	E3	E4	E5	E6	E7	E8
Substream: MIXED																				
Mole Flow kmol/hr																				
Mass Flow kg/hr																				
GLUCOSE	332.8	332.8	0.0	332.8	0.0	0.0	332.8	0.0	0.0	332.8	0.0	0.0	332.8	332.8	0.0	332.8	0.0	332.8	12.3	320.5
XYLOSE	4249.6	4249.6	0.0	4249.6	0.0	0.0	4249.6	0.0	0.0	4249.6	0.0	0.0	4249.6	4249.6	0.0	4249.6	0.0	4249.6	157.0	4092.5
ARABINOSE	204.8	204.8	0.0	204.8	0.0	0.0	204.8	0.0	0.0	204.8	0.0	0.0	204.8	204.8	0.0	204.8	0.0	204.8	7.6	197.2
ETHANOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	226712.0	192398.0	34314.1	168260.0	24138.2	24138.2	138523.0	29737.4	29737.4	103491.0	35031.3	35031.3	103491.0	103491.0	0.0	103491.0	0.0	103481.0	3823.9	99657.1
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	998.4	904.7	93.7	836.3	68.4	68.4	746.3	90.0	90.0	628.3	118.0	118.0	628.3	628.3	0.0	628.3	0.0	628.3	23.2	605.1
FURFURAL	51.2	50.2	1.0	49.4	0.8	0.8	48.0	1.3	1.3	45.9	2.1	2.1	45.9	45.9	0.0	45.9	0.0	45.9	1.7	44.2
NAOH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	58.0	58.0	0.0	0.0	0.0	0.0
H2SO4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	71.1	0.0	0.0	0.0
HMF	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FORMIC ACID	179.2	144.5	34.7	123.4	21.1	21.1	100.3	23.1	23.1	75.6	24.7	24.7	75.6	75.6	0.0	75.6	0.0	75.6	2.8	72.8
MG-O LGSPNT	23270.3	23270.3	0.0	23270.3	0.0	0.0	23270.3	0.0	0.0	23270.3	0.0	0.0	23270.3	23270.3	0.0	23270.3	0.0	23270.3	859.9	22410.4
Total Flow kmol/hr	13670.4	11763.4	1907.0	10421.9	1341.5	1341.5	8769.2	1652.7	1652.7	6822.1	1947.1	1947.1	6822.1	6822.1	1.5	6823.6	0.7	6821.6	252.1	6569.5
Total Flow kg/hr	255999.0	221555.0	34443.4	197327.0	24228.6	24228.6	167475.0	29851.8	29851.8	132299.0	35176.1	35176.1	132299.0	132299.0	58.0	132357.0	71.1	132288.0	4888.4	127400.0
Total Flow cum/hr	255.0	216.3	365999.0	193.4	138197.0	24.7	164.6	95445.4	30.8	129.9	65677.1	36.6	129.9	124.4	0.1	124.4	0.0	170.0	4.6	119.7
Temperature C	80.0	54.8	54.8	69.7	69.7	67.2	85.3	85.3	82.0	102.1	102.1	97.3	102.1	30.0	25.0	30.0	25.0	28.2	30.0	30.0
Pressure atm	2.0	0.1	0.1	0.3	0.3	0.3	0.5	0.5	0.5	0.9	0.9	0.9	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Vapor Frac	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Liquid Frac	1.0	1.0	0.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Solids																				
Mass Flow kg/hr																				
ASH	2912.1	2912.1	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	2912.1	0.0	2912.1	0.0	2912.1	107.6	2804.5
Total Flow kmol/hr	51.9	51.9	0.0	51.9	0.0	0.0	51.9	0.0	0.0	51.9	0.0	0.0	51.9	51.9	0.0	51.9	0.0	51.9	1.9	50.0
Total Flow kg/hr	2912.1	2912.1	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	2912.1	0.0	2912.1	0.0	2912.1	107.6	2804.5
Total Flow cum/hr	0.9	0.9	0.0	0.9	0.0	0.0	0.9	0.0	0.0	0.9	0.0	0.0	0.9	0.9	0.0	0.9	0.0	0.9	0.0	0.8
Temperature C	80.0	54.8		69.7			85.3			102.1			102.1	30.0	25.0	30.0		28.2	30.0	30.0
Pressure atm	2.0	0.1	0.1	0.3	0.3	0.3	0.5	0.5	0.5	0.9	0.9	0.9	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

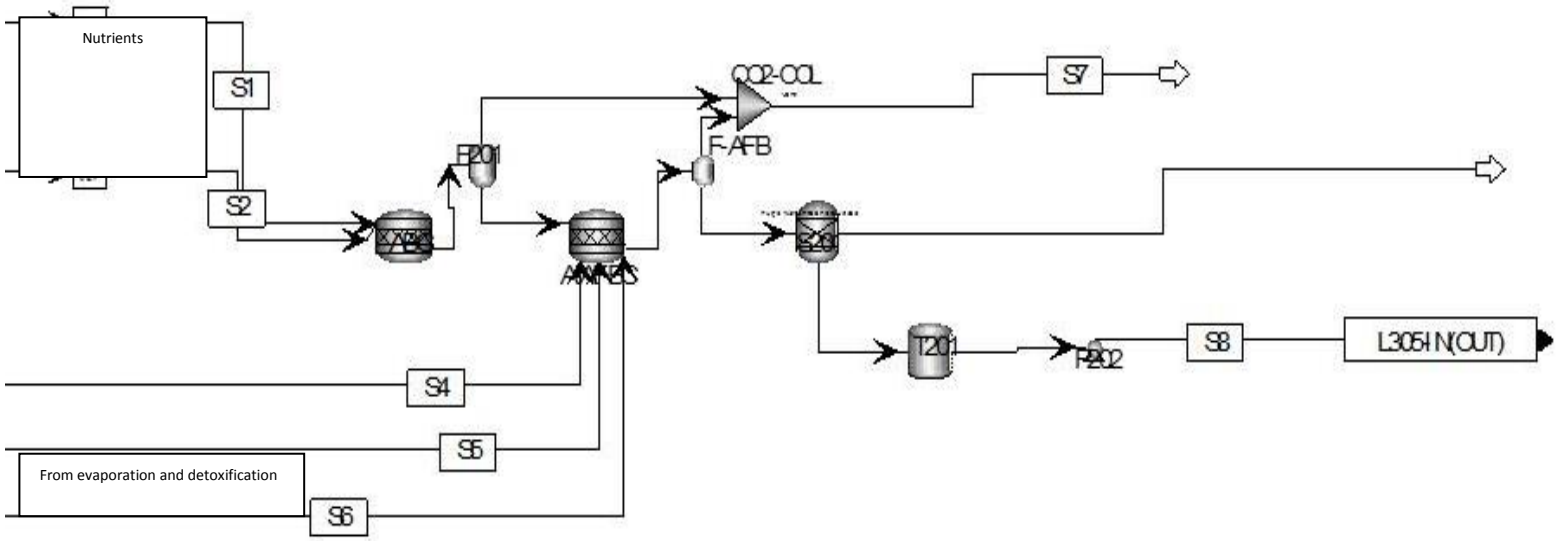
2.4 5 –EFFECT CONCENTRATION AND DETOXIFICATION





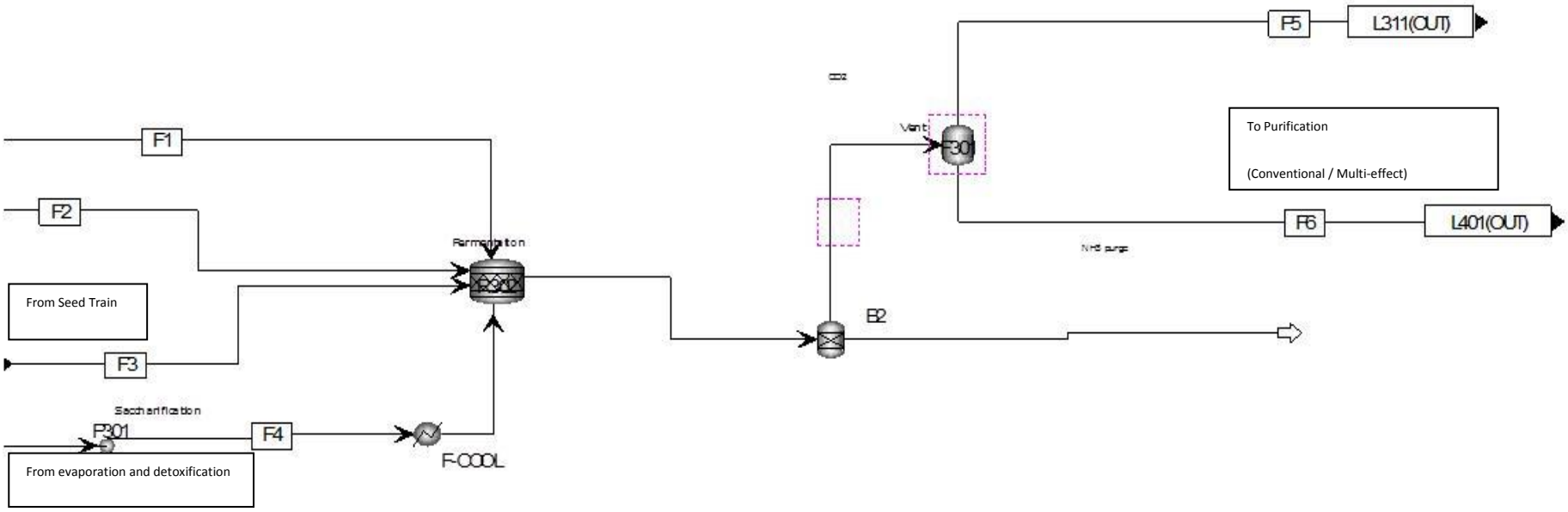
	MF	E1C	E1V	E2C	E2V	E2VC	E3C	E3V	E3VC	E4C	E4V	E4VC	E5C	E5V	E5VC	E1	E2	E3	E4	E5	E6	E7	E8	E9	E10
Substream: MIXED																									
Mass Flow kg/hr																									
GLUCOSE	332.8	332.8	0.0	332.8	0.0	0.0	332.8	0.0	0.0	332.8	0.0	0.0	332.8	0.0	0.0	0.0	332.8	332.8	0.0	332.8	0.0	332.8	332.8	11.2	321.6
XYLOSE	4249.6	4249.6	0.0	4249.6	0.0	0.0	4249.6	0.0	0.0	4249.6	0.0	0.0	4249.6	0.0	0.0	0.0	4249.6	4249.6	0.0	4249.6	0.0	4249.6	4249.6	142.9	4106.7
ARABINOSE	204.8	204.8	0.0	204.8	0.0	0.0	204.8	0.0	0.0	204.8	0.0	0.0	204.8	0.0	0.0	0.0	204.8	204.8	0.0	204.8	0.0	204.8	204.8	6.9	197.9
XYLITOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
EXTRACT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ETHANOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	226712.0	192502.0	34210.2	168467.0	24034.8	24034.8	138832.0	29635.4	29635.4	103900.0	34931.5	34931.5	64406.8	39493.7	39493.7	1198.9	63207.9	63207.9	0.0	63207.9	0.0	63207.9	63201.6	2125.6	61076.0
N2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	998.4	905.0	93.4	836.9	68.1	68.1	747.3	89.6	89.6	629.9	117.4	117.4	471.2	158.6	158.6	4.9	466.4	466.4	0.0	466.4	0.0	466.4	466.4	15.7	450.7
FURFURAL	51.2	50.2	1.0	49.4	0.8	0.8	48.1	1.3	1.3	45.9	2.1	2.1	42.2	3.7	3.7	0.1	42.1	42.1	0.0	42.1	0.0	42.1	42.1	1.4	40.7
NAOH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	40.0	40.0	0.0	40.0	0.0	0.0	0.0
H2SO4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	49.0	49.0	0.0	0.0	0.0
HMF	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FORMIC ACID	179.2	144.6	34.6	123.6	21.1	21.1	100.6	23.0	23.0	75.9	24.7	24.7	49.0	26.9	26.9	0.9	48.2	48.2	0.0	48.2	0.0	48.2	48.2	1.6	46.6
MG-O LGSPNT	23270.3	23270.3	0.0	23270.3	0.0	0.0	23270.3	0.0	0.0	23270.3	0.0	0.0	23270.3	0.0	0.0	0.0	23270.3	23270.3	0.0	23270.3	0.0	23270.3	23270.3	782.6	22487.6
Total Flow kmol/hr	13670.4	11769.1	1901.3	10433.4	1335.7	1335.7	8786.4	1647.0	1647.0	6844.9	1941.5	1941.5	4649.4	2195.5	2195.5	66.6	4582.7	4582.7	1.0	4583.7	0.5	4584.2	4582.4	154.1	4428.3
Total Flow kg/hr	255999.0	221659.0	34339.1	197535.0	24124.8	24124.8	167785.0	29749.3	29749.3	132710.0	35075.7	35075.7	93026.7	39682.9	39682.9	1204.7	91822.0	91822.0	40.0	91862.0	49.0	91911.0	91815.7	3087.9	88727.7
Total Flow cum/hr	255.0	216.4	364889.0	193.6	137604.0	24.6	164.9	95115.9	30.7	130.3	65486.7	36.5	89.9	51567.2	41.7	2068.7	88.0	83.7	0.1	83.8	0.0	83.8	123.5	2.8	80.9
Temperature C	80.0	54.8	54.8	69.7	69.7	67.2	85.3	85.3	82.0	102.1	102.1	97.3	116.6	116.6	108.7	107.7	107.7	30.0	25.0	30.0	25.0	30.0	28.3	30.0	30.0
Pressure atm	2.0	0.1	0.1	0.3	0.3	0.3	0.5	0.5	0.5	0.9	0.9	0.9	1.4	1.4	1.4	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Vapor Frac	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Liquid Frac	1.0	1.0	0.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
SOLIDS																									
Mass Flow kg/hr																									
ASH	2912.1	2912.1	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	0.0	2912.1	2912.1	0.0	2912.1	0.0	2912.1	2912.1	97.9	2814.1
Total Flow kmol/hr	51.9	51.9	0.0	51.9	0.0	0.0	51.9	0.0	0.0	51.9	0.0	0.0	51.9	0.0	0.0	0.0	51.9	51.9	0.0	51.9	0.0	51.9	51.9	1.7	50.2
Total Flow kg/hr	2912.1	2912.1	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	2912.1	0.0	0.0	0.0	2912.1	2912.1	0.0	2912.1	0.0	2912.1	2912.1	97.9	2814.1
Total Flow cum/hr	0.9	0.9	0.0	0.9	0.0	0.0	0.9	0.0	0.0	0.9	0.0	0.0	0.9	0.0	0.0	0.0	0.9	0.9	0.0	0.9	0.0	0.9	0.9	0.0	0.8
Temperature C	80.0	54.8		69.7			85.3			102.1			116.6				107.7	30.0	25.0	30.0		30.0	28.3	30.0	30.0
Pressure atm	2.0	0.1	0.1	0.3	0.3	0.3	0.5	0.5	0.5	0.9	0.9	0.9	1.4	1.4	1.4	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

2.5 SEED TRAIN



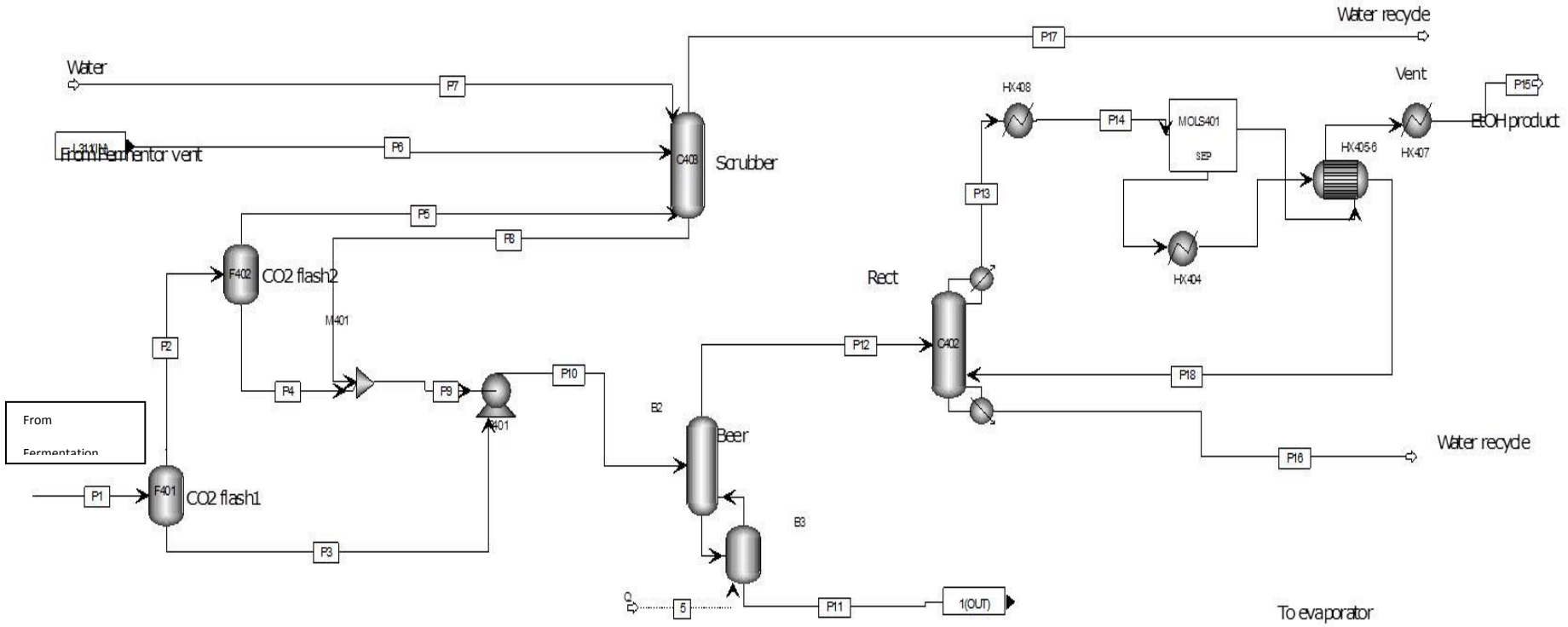
	S1	S2	S3	S4	S5	S6	S7	S8
Substream: MIXED								
Mass Flow kg/hr								
GLUCOSE	1.3	0.0	0.0	0.0	11.2	147.0	0.0	0.0
XYLOSE	0.0	0.0	0.0	0.0	142.9	441.1	0.0	0.0
ARABINOSE	0.0	0.0	0.0	0.0	6.9	0.0	0.0	6.9
XYLITOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
EXTRACT	0.0	0.0	0.0	0.0	0.0	14.7	0.0	0.0
ETHANOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	0.0	0.0	0.5	0.0	2125.6	6175.8	53.1	8471.5
N2	0.0	5.1	5.1	1608.1	0.0	0.0	1613.2	0.1
CO2	0.0	0.0	1.3	0.0	0.0	0.0	543.3	2.0
O2	0.0	1.5	0.5	453.6	0.0	0.0	58.6	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	0.0	0.0	0.0	0.0	15.7	0.0	0.1	15.6
NH4SO4	0.0	0.0	0.0	0.0	0.0	5.9	0.0	0.0
FURFURAL	0.0	0.0	0.0	0.0	1.4	0.0	0.0	1.4
H2SO4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HMF	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MGSO4	0.0	0.0	0.0	0.0	0.0	2.9	0.0	0.0
(NH4)3-PO4	0.0	0.0	0.0	0.0	0.0	11.8	0.0	0.0
FORMIC ACID	0.0	0.0	0.0	0.0	1.6	0.0	0.0	0.0
MG-O LGSPNT	0.0	0.0	0.0	0.0	782.6	0.0	0.0	782.6
Total Flow kmol/hr	0.0	0.2	0.3	71.6	154.1	346.8	74.7	505.4
Total Flow kg/hr	1.3	6.6	7.5	2061.7	3087.9	6799.3	2268.2	9280.1
Total Flow cum/hr	0.0	5.6	5.9	1750.4	2.8	6.7	1856.3	9.1
Temperature C	30.0	25.0	30.0	25.0	30.0	25.0	30.0	30.0
Pressure atm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.1
Vapor Frac	0.0	1.0	0.9	1.0	0.0	0.0	1.0	0.0
Liquid Frac	1.0	0.0	0.1	0.0	1.0	1.0	0.0	1.0
SOLIDS								
Mass Flow kg/hr								
YEAST	0.0	0.0	0.4	0.0	0.0	0.0	0.0	371.9
ASH	0.0	0.0	0.0	0.0	97.9	0.0	0.0	97.9
Total Flow kmol/hr	0.0	0.0	0.0	0.0	1.7	0.0	0.0	17.8
Total Flow kg/hr	0.0	0.0	0.4	0.0	97.9	0.0	0.0	469.8
Total Flow cum/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3
Temperature C			30.0		30.0			30.0
Pressure atm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.1

2.6 FERMENTATION



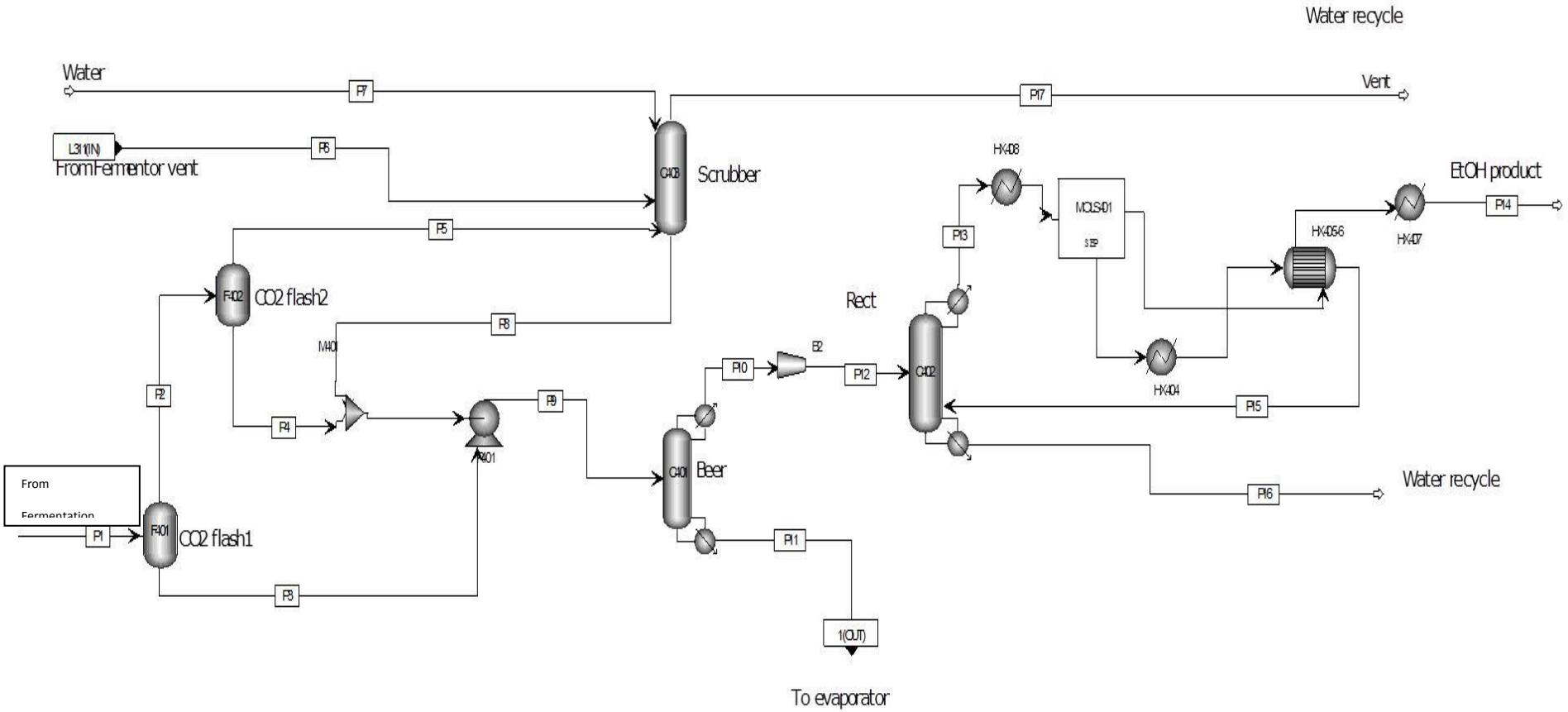
	F1	F2	F3	F4	F5	F6
Substream: MIXED						
Mass Flow kg/hr						
GLUCOSE	0.0	0.0	0.0	321.6	0.0	67.7
XYLOSE	0.0	0.0	0.0	4106.7	0.0	800.9
ARABINOSE	0.0	0.0	6.9	197.9	0.0	20.5
XYLITOL	0.0	0.0	0.0	0.0	0.0	109.5
CSL	1054.1	0.0	0.0	0.0	0.0	0.0
PROTEIN	0.0	0.0	0.0	0.0	0.0	0.0
ETHANOL	0.0	0.0	0.0	0.0	4.6	1833.5
H2O	10.6	0.0	8471.5	61076.0	21.2	69534.6
N2	0.0	0.0	0.1	0.0	0.1	0.0
CO2	0.0	0.0	2.0	0.0	1630.7	130.1
O2	0.0	0.0	0.0	0.0	11.5	0.0
NH3	0.0	191.6	0.0	0.0	0.0	0.0
FURFURAL	0.0	0.0	15.6	450.7	0.1	466.2
GLYCEROL	0.0	0.0	0.0	0.0	0.0	0.0
FURFURAL	0.0	0.0	1.4	40.7	0.0	42.1
FORMIC ACID	0.0	0.0	0.0	46.6	0.0	46.5
MG-O LGSPNT	0.0	0.0	782.6	22487.6	0.0	23270.3
Total Flow kmol/hr	6.0	11.3	505.4	4428.3	38.7	4951.7
Total Flow kg/hr	1064.7	191.6	9280.1	88727.7	1668.3	96322.0
Total Flow cum/hr	0.1	273.3	9.1	80.9	870.4	90.6
Temperature C	25.0	25.0	30.0	30.0	30.0	30.0
Pressure atm	1.0	1.0	1.1	1.2	1.1	1.1
Vapor Frac	0.0	1.0	0.0	0.0	1.0	0.0
Liquid Frac	1.0	0.0	1.0	1.0	0.0	1.0
SOLIDS						
Mass Flow kg/hr						
YEAST	0.0	0.0	371.9	0.0	0.0	404.6
ASH	0.0	0.0	97.9	2814.1	0.0	2912.1
Total Flow kmol/hr	0.0	0.0	17.8	50.2	0.0	69.3
Total Flow kg/hr	0.0	0.0	469.8	2814.1	0.0	3316.6
Total Flow cum/hr	0.0	0.0	0.3	0.8	0.0	1.1
Temperature C			30.0	30.0		30.0
Pressure atm	1.0	1.0	1.1	1.2	1.1	1.1

2.7 CONVENTIONAL DISTILLATION (DEMONSTRATED FOR SCENARIO OF FERMENTING SUBSTRATE WITH 30% SOLIDS)



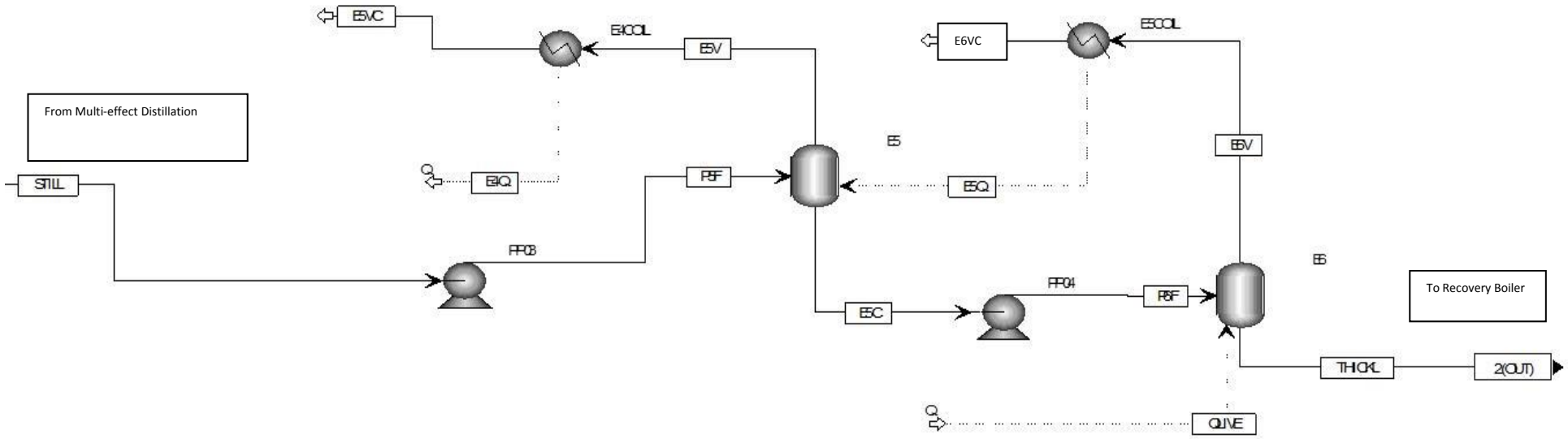
	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	P11	P12	P13	P14	P15	P16	P17	P18
Substream: MIXED																		
Mass Flow kg/hr																		
GLUCOSE	67.7	0.0	67.7	0.0	0.0	0.0	0.0	0.0	0.0	67.7	67.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLOSE	800.9	0.0	800.9	0.0	0.0	0.0	0.0	0.0	0.0	800.9	800.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARABINOSE	20.5	0.0	20.5	0.0	0.0	0.0	0.0	0.0	0.0	20.5	20.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GALACTOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MANNOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLITOL	109.5	0.0	109.5	0.0	0.0	0.0	0.0	0.0	0.0	109.5	109.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
EXTRACT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ETHANOL	1833.5	9.6	1823.9	5.7	3.9	4.6	0.0	8.6	14.2	1838.1	5.6	1832.5	2288.6	2288.6	1830.9	1.6	0.0	457.7
H2O	69534.6	53.4	69481.2	50.5	2.9	21.2	2491.9	2504.6	2555.2	72036.4	57477.4	14559.0	207.3	207.3	1.0	14558.0	11.3	206.3
N2	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0
CO2	130.1	111.3	18.8	0.1	111.3	1630.7	0.0	4.3	4.4	23.2	0.0	23.2	23.2	23.2	23.2	0.0	1737.7	0.0
O2	0.0	0.0	0.0	0.0	0.0	11.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11.5	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	466.2	0.2	466.0	0.2	0.0	0.1	0.0	0.1	0.3	466.3	415.9	50.4	0.0	0.0	0.0	50.4	0.0	0.0
FURFURAL	42.1	0.0	42.1	0.0	0.0	0.0	0.0	0.0	0.0	42.1	41.0	1.1	0.0	0.0	0.0	1.1	0.0	0.0
HMF	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FORMIC ACID	46.5	0.0	46.5	0.0	0.0	0.0	0.0	0.0	0.1	46.6	37.8	8.7	0.0	0.0	0.0	8.7	0.0	0.0
MG-O LGSPNT	23270.3	0.0	23270.3	0.0	0.0	0.0	0.0	0.0	0.0	23270.3	23270.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	4951.7	5.7	4946.0	2.9	2.8	38.7	138.3	139.3	142.3	5088.2	4238.7	849.5	61.7	61.7	40.3	809.2	40.5	21.4
Total Flow kg/hr	96322.0	174.7	96147.3	56.5	118.1	1668.3	2491.9	2517.7	2574.2	98721.5	82246.6	16475.0	2519.1	2519.1	1855.1	14619.8	1760.6	664.0
Total Flow cum/hr	205.4	201.6	136.6	0.1	64.4	870.4	2.5	2.5	2.6	95.9	80.1	25017.1	1779.2	1441.0	6.6	16.0	928.2	0.8
Temperature C	86.0	84.1	84.1	38.0	38.0	30.0	13.0	19.4	19.8	83.7	113.7	106.5	78.2	120.0	25.0	101.4	13.8	80.0
Pressure atm	1.1	0.8	0.8	1.1	1.1	1.1	2.0	1.0	1.1	1.7	1.2	1.1	1.0	1.4	1.3	1.1	1.0	1.5
Vapor Frac	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	1.0	0.0
Liquid Frac	1.0	0.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	0.0	1.0	1.0	0.0	1.0
SOLIDS																		
Mass Flow kg/hr																		
YEAST	404.6	0.0	404.6	0.0	0.0	0.0	0.0	0.0	0.0	404.6	404.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH	2912.1	0.0	2912.1	0.0	0.0	0.0	0.0	0.0	0.0	2912.1	2912.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	69.3	0.0	69.3	0.0	0.0	0.0	0.0	0.0	0.0	69.3	69.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	3316.6	0.0	3316.6	0.0	0.0	0.0	0.0	0.0	0.0	3316.6	3316.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow cum/hr	1.1	0.0	1.1	0.0	0.0	0.0	0.0	0.0	0.0	1.1	1.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Temperature C	86.0		84.1							83.7	113.7							
Pressure atm	1.1	0.8	0.8	1.1	1.1	1.1	2.0	1.0	1.1	1.7	1.2			1.4	1.3	1.1		1.5

2.8 MULTI-EFFECT DISTILLATION (DEMONSTRATED FOR SCENARIO OF FERMENTING SUBSTRATE WITH 20% SOLIDS)



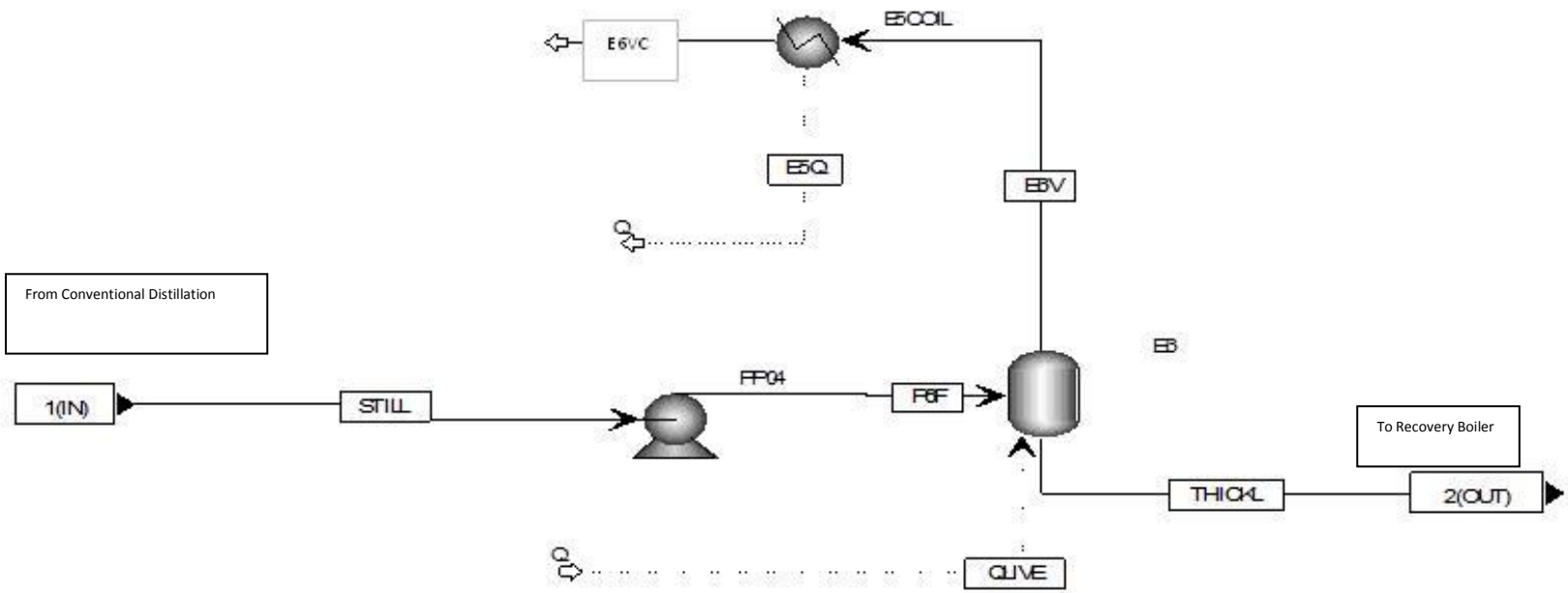
	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	P11	P12	P13	P14	P15	P16	P17
Substream: MIXED																	
Mass Flow kg/hr																	
GLUCOSE	43.7	0.0	43.7	0.0	0.0	0.0	0.0	0.0	43.7	0.0	43.7	0.0	0.0	0.0	0.0	0.0	0.0
XYLOSE	517.1	0.0	517.1	0.0	0.0	0.0	0.0	0.0	517.1	0.0	517.1	0.0	0.0	0.0	0.0	0.0	0.0
ARABINOSE	20.5	0.0	20.5	0.0	0.0	0.0	0.0	0.0	20.5	0.0	20.5	0.0	0.0	0.0	0.0	0.0	0.0
GALACTOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MANNOSE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XYLITOL	70.7	0.0	70.7	0.0	0.0	0.0	0.0	0.0	70.7	0.0	70.7	0.0	0.0	0.0	0.0	0.0	0.0
EXTRACT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ETHANOL	2010.5	13.8	1996.7	8.6	5.2	4.5	0.0	9.7	2014.9	2008.9	6.0	2008.9	2507.4	2005.9	501.5	3.0	0.0
H2O	113500.0	95.5	113405.0	91.2	4.3	24.6	2651.0	2667.5	116164.0	23415.5	92748.1	23415.5	222.8	1.1	221.7	23414.4	12.4
N2	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2
CO2	191.8	166.8	25.0	0.1	166.7	1738.2	0.0	4.6	29.7	29.7	0.0	29.7	29.7	29.7	0.0	0.0	1900.3
O2	0.0	0.0	0.0	0.0	0.0	7.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	7.4
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LACTIC ACID	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	628.2	0.3	627.9	0.3	0.0	0.1	0.0	0.1	628.3	73.5	554.7	73.5	0.0	0.0	0.0	73.5	0.0
FURFURAL	45.9	0.0	45.9	0.0	0.0	0.0	0.0	0.0	45.9	1.1	44.8	1.1	0.0	0.0	0.0	1.1	0.0
H2SO4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HMF	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FORMIC ACID	72.8	0.1	72.7	0.1	0.0	0.0	0.0	0.0	72.8	18.5	54.3	18.5	0.0	0.0	0.0	18.5	0.0
MG-O LGSPNT	23270.3	0.0	23270.3	0.0	0.0	0.0	0.0	0.0	23270.3	0.0	23270.3	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	7398.4	9.4	7389.0	5.3	4.1	41.2	147.2	148.4	7542.7	1345.7	6197.0	1345.7	67.5	44.3	23.2	1301.4	44.1
Total Flow kg/hr	140372.0	276.5	140095.0	100.3	176.2	1775.0	2651.0	2681.9	142878.0	25547.2	117330.0	25547.2	2759.9	2036.8	723.2	23510.4	1920.3
Total Flow cum/hr	318.6	331.8	189.2	0.1	96.1	926.7	2.7	2.7	141.7	204798.0	159.8	59191.5	1944.9	9.2	0.9	25.7	1011.8
Temperature C	86.0	84.0	84.0	38.0	38.0	30.0	13.0	20.1	84.4	60.7	62.0	291.1	78.2	25.0	80.0	101.4	13.9
Pressure atm	1.1	0.8	0.8	1.1	1.1	1.1	2.0	1.0	1.7	0.2	0.2	1.1	1.0	1.3	1.5	1.1	1.0
Vapor Frac	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	1.0
Liquid Frac	1.0	0.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0
Solid Frac	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SOLIDS																	
Mass Flow kg/hr																	
YEAST	572.20751	0	572.20751	0	0	0	0	0	572.20751	0	572.20751	0	0	0	0	0	0
ASH	2912.063	0	2912.063	0	0	0	0	0	2912.063	0	2912.063	0	0	0	0	0	0
Total Flow kmol/hr	76.50629	0	76.50629	0	0	0	0	0	76.50629	0	76.50629	0	0	0	0	0	0
Total Flow kg/hr	3484.27	0	3484.27	0	0	0	0	0	3484.27	0	3484.27	0	0	0	0	0	0
Total Flow cum/hr	1.25202	0	1.25202	0	0	0	0	0	1.25202	0	1.25202	0	0	0	0	0	0
Temperature C	86		83.96904						84.37548		62.0205						
Pressure atm	1.1	0.83	0.83	1.1	1.1	1.1	2.042931	1.020689	1.7		0.18	1.05		1.26	1.5	1.05	

2.9 POST DISTILLATION CONCENTRATION OF FERMENTATION RESIDUE OF 20%-SOLID SUBSTRATE



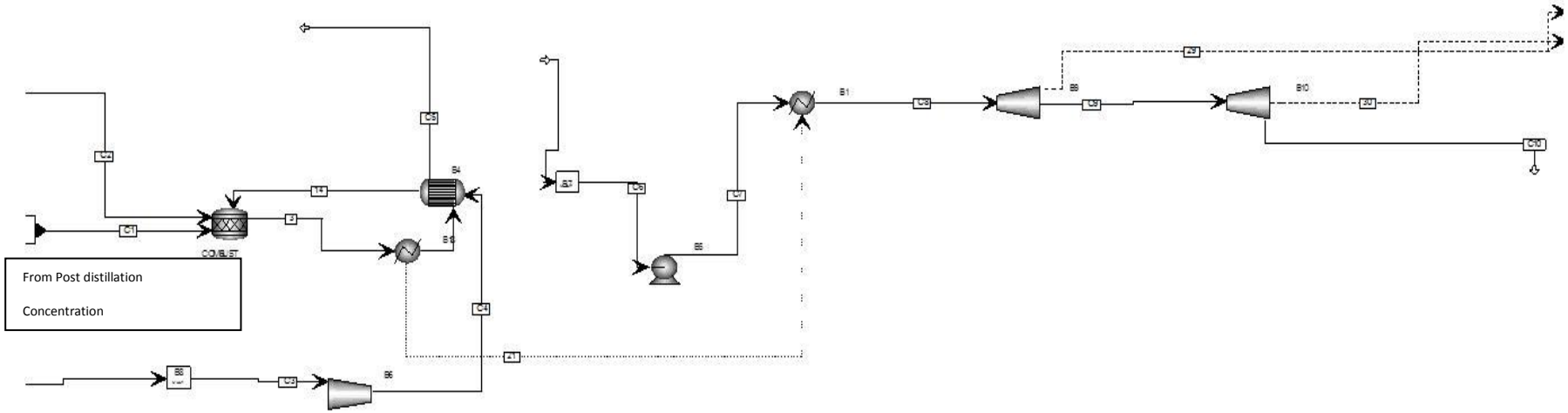
	STILL	E5C	E5V	E5VC	E6V	E6VC	THICKL
Substream: MIXED							
GLUCOSE	43.7	43.7	0.0	0.0	0.0	0.0	43.7
XYLOSE	517.1	517.1	0.0	0.0	0.0	0.0	517.1
ARABINOSE	20.5	20.5	0.0	0.0	0.0	0.0	20.5
XYLITOL	70.7	70.7	0.0	0.0	0.0	0.0	70.7
ETHANOL	6.0	1.5	4.5	4.5	1.3	1.3	0.2
H2O	92748.1	60799.5	31948.7	31948.7	41360.0	41360.0	19439.5
ACETIC ACID	554.7	430.6	124.2	124.2	229.2	229.2	201.3
FURFURAL	44.8	41.7	3.2	3.2	10.6	10.6	31.1
FORMIC ACID	54.3	37.0	17.4	17.4	22.9	22.9	14.0
MG-O LGSPNT	23270.3	23270.3	0.0	0.0	0.0	0.0	23270.3
Total Flow kmol/hr	6197.0	4421.0	1776.0	1776.0	2300.3	2300.3	2120.7
Total Flow kg/hr	117330.0	85232.4	32097.9	32097.9	41624.0	41624.0	43608.3
Total Flow cum/hr	159.8	83.7	42251.7	33.7	34652.5	44.3	40.9
Temperature C	62.0	116.5	116.5	108.3	148.5	124.8	148.5
Pressure atm	0.2	1.3	1.3	1.3	2.3	2.3	2.3
SOLID							
Mass Flow kg/hr							
YEAST	572.2	572.2	0.0	0.0	0.0	0.0	572.2
ASH	2912.1	2912.1	0.0	0.0	0.0	0.0	2912.1
Total Flow kmol/hr	76.5	76.5	0.0	0.0	0.0	0.0	76.5
Total Flow kg/hr	3484.3	3484.3	0.0	0.0	0.0	0.0	3484.3
Total Flow cum/hr	1.3	1.3	0.0	0.0	0.0	0.0	1.3
Temperature C	62.0	116.5					148.5
Pressure atm	0.2	1.3	1.3	1.3	2.3	2.3	2.3

2.10 POST DISTILLATION CONCENTRATION OF FERMENTATION RESIDUE OF 30%-SOLID SUBSTRATE



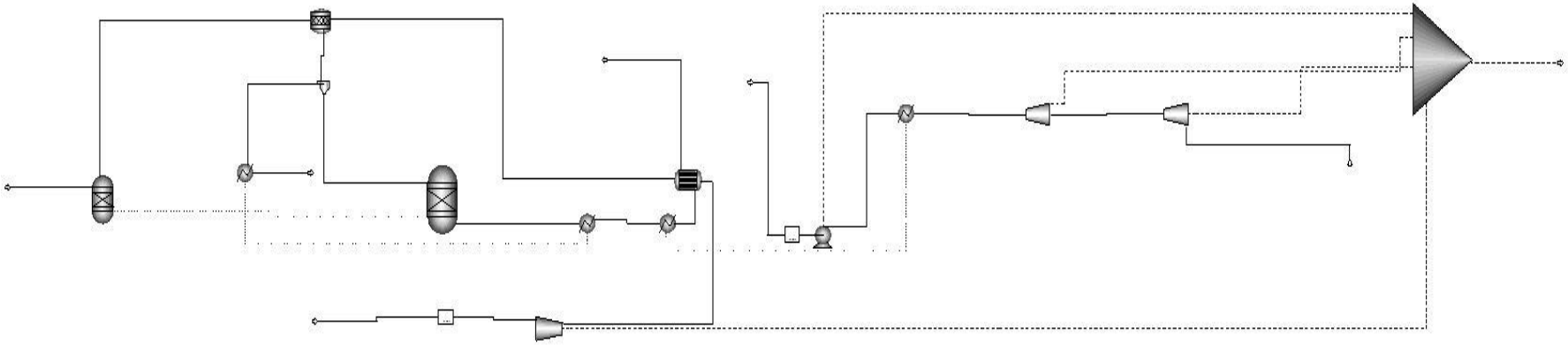
	E6V	E6VC	THICKL
Substream: MIXED			
Mass Flow kg/hr			
GLUCOSE	0.0	0.0	67.7
XYLOSE	0.0	0.0	800.9
ARABINOSE	0.0	0.0	20.5
XYLITOL	0.0	0.0	109.5
ETHANOL	4.8	4.8	0.8
H2O	37734.9	37734.9	19742.5
ACETIC ACID	210.4	210.4	205.5
FURFURAL	9.5	9.5	31.4
FORMIC ACID	22.6	22.6	15.3
MG-O LGSPNT	0.0	0.0	23270.3
Total Flow kmol/hr	2098.8	2098.8	2139.9
Total Flow kg/hr	37982.3	37982.3	44264.3
Total Flow cum/hr	32918.1	40.4	41.3
Temperature C	146.6	123.3	146.6
Pressure atm	2.2	2.2	2.2
Vapor Frac	1.0	0.0	0.0
Liquid Frac	0.0	1.0	1.0
Solid Frac	0.0	0.0	0.0
Solids			
Mass Flow kg/hr			
YEAST	0.0	0.0	404.6
ASH	0.0	0.0	2912.1
Total Flow kmol/hr	0.0	0.0	69.3
Total Flow kg/hr	0.0	0.0	3316.6
Total Flow cum/hr	0.0	0.0	1.1
Temperature C			146.6
Pressure atm	2.2	2.2	2.2

2.11 RECOVERY BOILER FIRED WITH THICKENED FERMENTATION RESIDUE



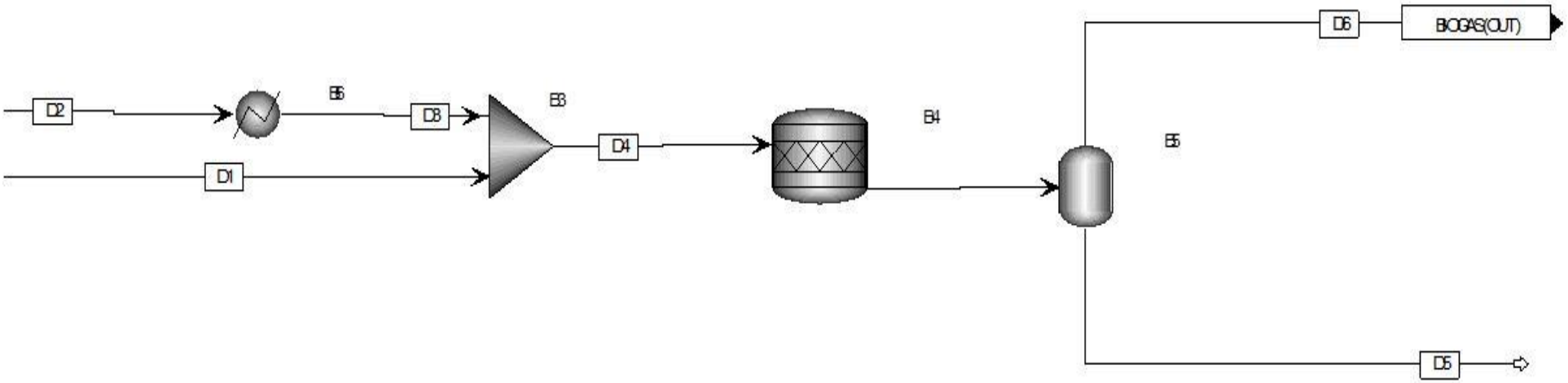
	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10
Substream: MIXED										
Mass Flow kg/hr										
GLUCOSE	67.7	0.0	0.0	0.0	0.7	0.0	0.0	0.0	0.0	0.0
XYLOSE	800.9	0.0	0.0	0.0	8.0	0.0	0.0	0.0	0.0	0.0
ARABINOSE	20.5	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0
XYLITOL	109.5	0.0	0.0	0.0	1.1	0.0	0.0	0.0	0.0	0.0
ETHANOL	0.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	19742.5	79.2	0.0	0.0	27797.6	132237.0	132237.0	132237.0	132237.0	132237.0
N2	0.0	0.0	160948.0	160948.0	162510.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	1403.4	2988.4	2988.4	53808.7	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	49522.3	49522.3	8484.1	0.0	0.0	0.0	0.0	0.0
CH4	0.0	518.2	0.0	0.0	5.2	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	205.5	0.0	0.0	0.0	2.1	0.0	0.0	0.0	0.0	0.0
SO2	0.0	0.0	0.0	0.0	7363.9	0.0	0.0	0.0	0.0	0.0
FURFURAL	31.4	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.0
H2SO4	0.0	0.0	0.0	0.0	113.9	0.0	0.0	0.0	0.0	0.0
FORMIC ACID	15.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MG-O LGSPNT	23270.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	2139.9	71.1	7360.9	7360.9	8948.4	7340.3	7340.3	7340.3	7340.3	7340.3
Total Flow kg/hr	44264.3	2005.8	213458.0	213458.0	260095.0	132237.0	132237.0	132237.0	132237.0	132237.0
Total Flow cum/hr	41.3	1805.4	179995.0	177626.0	294123.0	132.6	136.4	8429.9	14675.3	36989.5
Temperature C	146.6	37.3	25.0	27.0	135.8	25.0	49.0	445.0	358.1	227.2
Pressure atm	2.2	1.0	1.0	1.0	1.0	1.0	48.4	48.4	24.7	7.9
Vapor Frac	0.0	1.0	1.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0
Liquid Frac	1.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
SOLIDS										
Mass Flow kg/hr										
YEAST	404.6	0.0	0.0	0.0	36.4	0.0	0.0	0.0	0.0	0.0
ASH	2912.1	0.0	0.0	0.0	2912.1	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	69.3	0.0	0.0	0.0	53.4	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	3316.6	0.0	0.0	0.0	2948.5	0.0	0.0	0.0	0.0	0.0
Total Flow cum/hr	1.1	0.0	0.0	0.0	0.9	0.0	0.0	0.0	0.0	0.0
Temperature C	146.6				135.8					
Pressure atm	2.2	1.0	1.0	1.0	1.0	1.0	48.4	48.4	24.7	7.9

2.12 COAL AND BARK COMBUSTION



	Flow-rate	Steam	Electricity
	Ton/hr	ton/hr	MW
Coal	8	58.0	6.0
	9	65.2	6.8
	10	72.6	7.5
	11	79.8	8.3
	12	87.0	9.0
	13	94.2	9.8
	14	101.5	10.6
	15	108.7	11.3
	16	116.0	12.1
	17	123.2	12.8
	18	130.5	13.6
	19	137.7	14.3
	20	145.0	15.1
	21	152.2	15.8
	22	159.5	16.6
	23	166.7	17.4
	24	174.0	18.1
	25	181.2	18.9
Biomass	17.3	75.8	10.6

2.13 BIODIGESTION



	D1	D2	D3	D4	D5	D6
Substream: MIXED						
Mass Flow kg/hr						
GLUCOSE	0.0	146.0	146.0	146.0	7.3	0.0
XYLOSE	0.0	1436.5	1436.5	1436.5	71.8	0.0
ARABINOSE	0.0	61.5	61.5	61.5	61.5	0.0
H2O	200706.0	63929.9	63929.9	264635.0	264556.0	79.2
CO2	0.0	0.0	0.0	0.0	134.8	1403.4
CH4	0.0	0.0	0.0	0.0	2.3	518.2
LACTIC ACID	0.0	0.0	0.0	0.0	0.0	0.0
ACETIC ACID	0.0	468.6	468.6	468.6	23.4	0.0
FURFURAL	0.0	15.4	15.4	15.4	15.4	0.0
FORMIC ACID	0.0	115.2	115.2	115.2	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	5.0
CA-O LGSPNT	0.0	10647.3	10647.3	10647.3	10647.3	0.0
Total Flow kmol/hr	11140.9	4040.4	4040.4	15181.2	15160.3	71.1
Total Flow kg/hr	200706.0	76820.4	76820.4	277526.0	275520.0	2005.8
Total Flow cum/hr	201.9	75.4	73.7	275.6	274.5	1805.4
Temperature C	35.0	80.0	40.0	36.3	37.3	37.3
Pressure atm	1.0	2.0	1.0	1.0	1.0	1.0
Vapor Frac	0.0	0.0	0.0	0.0	0.0	1.0
Liquid Frac	1.0	1.0	1.0	1.0	1.0	0.0
SOLIDS						
Mass Flow kg/hr						
ASH	0.0	852.8	852.8	852.8	852.8	0.0
Total Flow kmol/hr	0.0	15.2	15.2	15.2	15.2	0.0
Total Flow kg/hr	0.0	852.8	852.8	852.8	852.8	0.0
Total Flow cum/hr	0.0	0.3	0.3	0.3	0.3	0.0
Temperature C		80.0	40.0	36.3	37.3	
Pressure atm	1.0	2.0	1.0	1.0	1.0	1.0

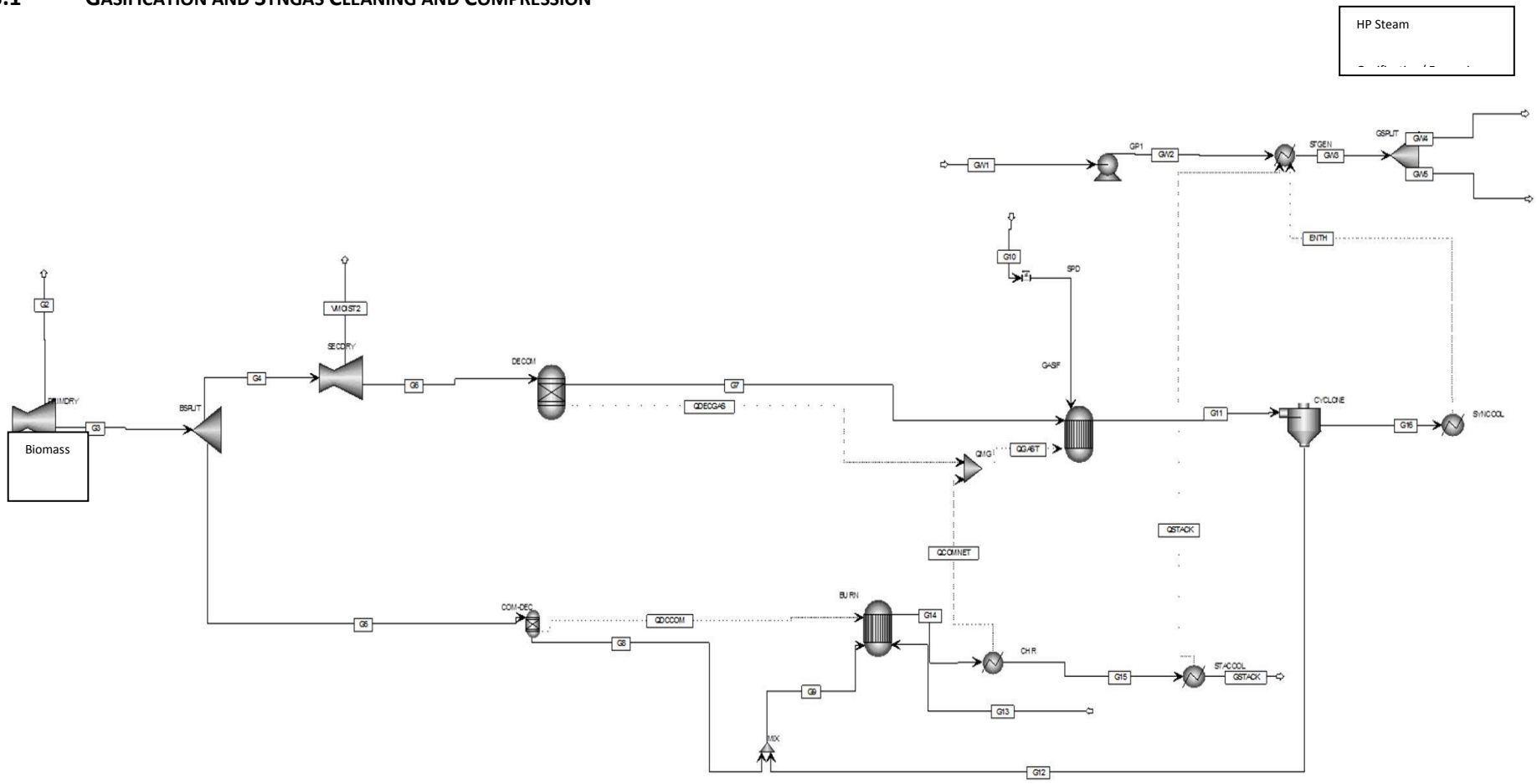
3. Appendix D3

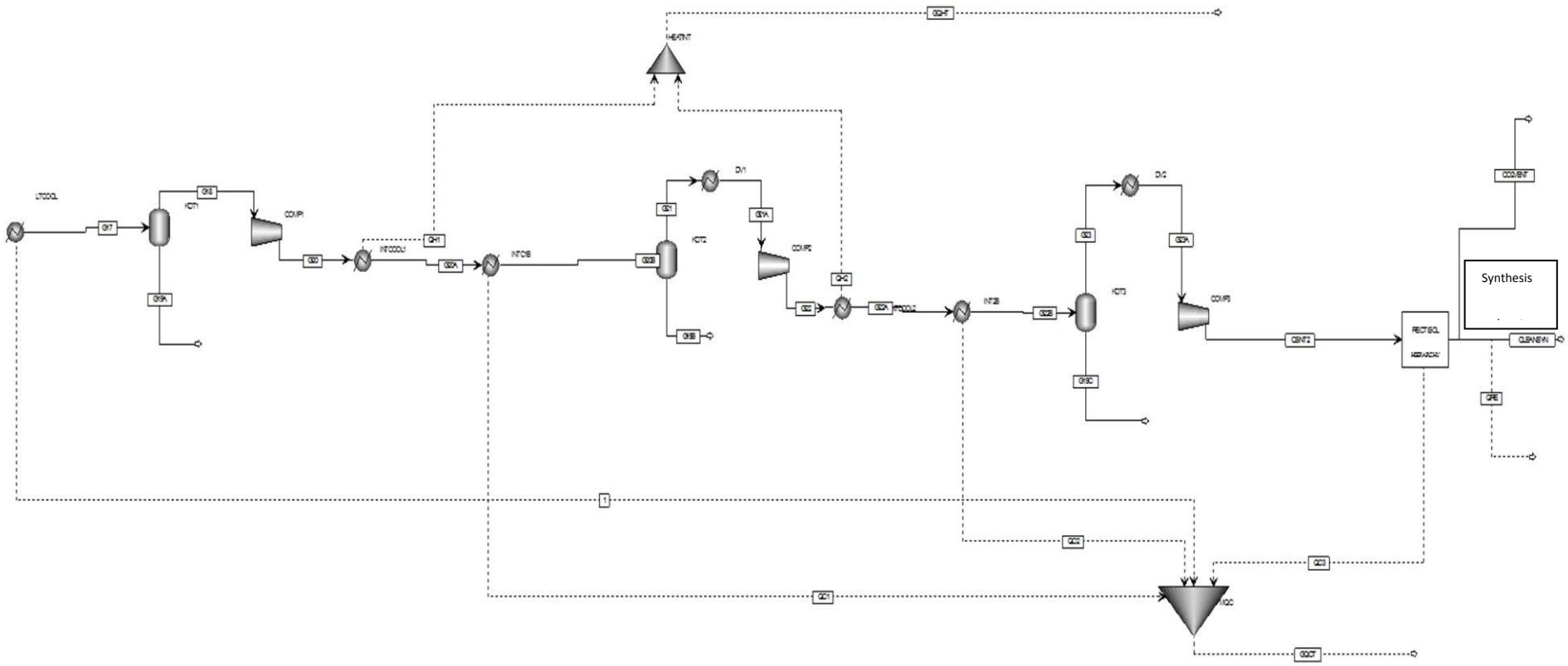
Table D 15: Configuration of flow sheets for Chapter 6 (MTOH-methanol synthesis; FT – Fischer-Tropsch synthesis; AD- advanced synthesis; CON – conventional synthesis)

	Overall Scenarios	Subsections/Component flow-sheets								
		Gasification and Syngas Conditioning	Conventional Methanol synthesis loop	Advanced Methanol Synthesis loop	Conventional Fischer-Tropsch synthesis loop	Advanced Fischer-Tropsch synthesis loop	Methanol Purification	Energy Generation Circuit	Gas Turbine Model	Rectisol Model
Flow Sheets	MTOH-CON	X	X				X	X	X	X
	MTOH-AD*	X		X			X	X	X	X
	FT-CON	X			X			X	X	X
	FT-AD	X				X		X	X	X

*full mass balance represented

3.1 GASIFICATION AND SYNGAS CLEANING AND COMPRESSION

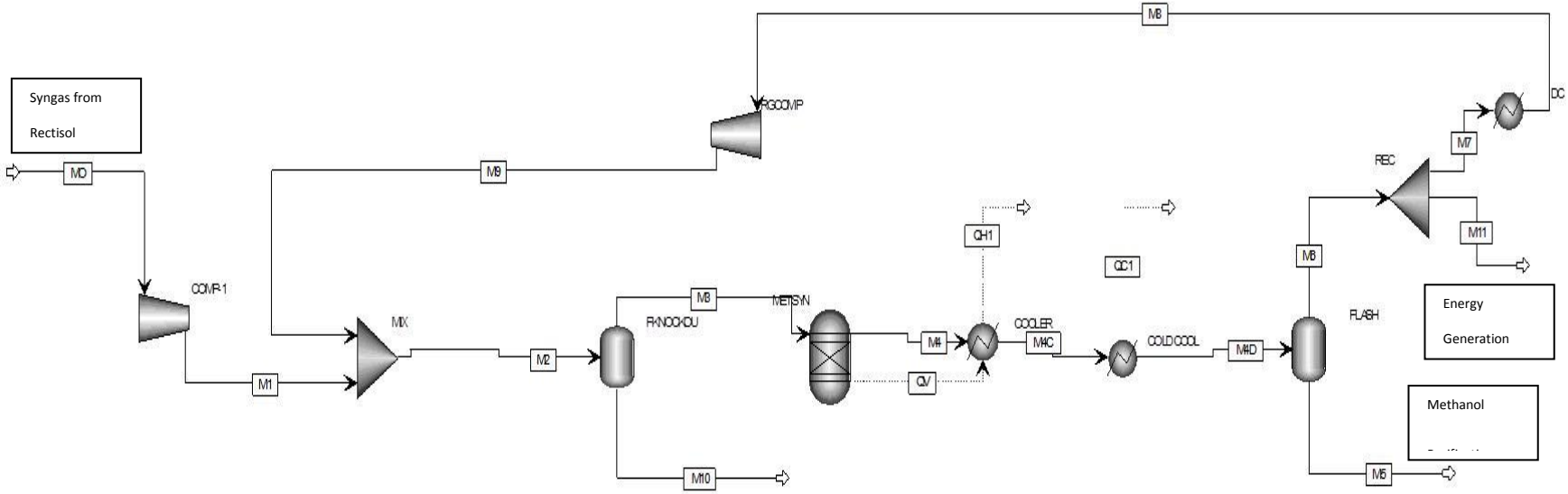




	G1	G2	G3	VMOIST2	G4	G5	G6	G7	G8	G9	G10	G11	G12	G13	G14	G15	G16	GSTACK	GW1	GW2	GW3	GW4	GW5
Substream: MIXED																							
Mass Flow kg/hr																							
H2O	45113.6	24609.9	20503.7	10019.6	11898.3	8605.4	1878.7	1878.7	8605.4	8605.4	35695.0	23916.7	0.0	0.0	21553.1	21553.1	23916.7	21553.1	94760.4	94760.4	94760.4	35695.0	59065.4
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15623.3	11299.5	11299.5	0.0	0.0	0.0	45055.0	15258.5	15258.5	0.0	15258.5	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	26.4	19.1	19.1	0.0	26.4	0.0	148306.0	148087.0	148087.0	26.4	148087.0	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	508.9	508.9	0.0	508.9	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	20555.2	0.0	0.0	40316.7	40316.7	20555.2	40316.7	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	22421.0	0.0	0.0	20.0	20.0	22421.0	20.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2003.9	1449.3	1449.3	0.0	3531.7	0.0	0.0	0.5	0.5	3531.7	0.5	0.0	0.0	0.0	0.0	0.0
SO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.6	0.0	0.0	0.0	0.0	1.6	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	2504.2	1366.1	1138.1	556.2	660.5	477.7	104.3	1587.5	1550.4	1550.4	1981.4	4348.1	0.0	6702.1	7893.5	7893.5	4348.1	7893.5	5260.0	5260.0	5260.0	1981.4	3278.6
Total Flow kg/hr	45113.6	24609.9	20503.7	10019.6	11898.3	8605.4	1878.7	19532.3	21373.4	21373.4	35695.0	70452.6	0.0	193361.0	225746.0	225746.0	70452.6	225746.0	94760.4	94760.4	94760.4	35695.0	59065.4
Total Flow l/min	792.8	432.5	360.3	176.1	209.1	151.2	33.0	624329.0	11895.5	59751.6	18654.1	7023830.0	0.0	4795090.0	19370600.0	13182800.0	7023830.0	5453190.0	1596.7	1603.9	49478.9	18638.0	30840.9
Temperature K	344.2	344.2	344.2	344.2	344.2	344.2	344.2	298.2	25.0	60.3	843.2	1181.2		523.2	1794.4	1221.2	1181.2	505.2	303.2	307.7	842.4	842.4	842.4
Pressure atm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	122.5	1.0		1.0	1.0	1.0	1.0	1.0	1.0	122.5	122.5	122.5	122.5
Vapor Frac	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.2	0.5	1.0	1.0		1.0	1.0	1.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0
Liquid Frac	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	0.8	0.5	0.0	0.0		0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
Substream: CISOLID																							
Mass Flow kg/hr																							
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15225.3	11011.7	11011.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASHO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2816.0	2036.6	4852.6	0.0	2816.0	2816.0	0.0	4852.6	4852.6	0.0	4852.6	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1317.8	953.1	1003.3	0.0	50.2	50.2	0.0	86.5	86.5	0.0	86.5	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	18041.3	13048.3	15864.3	0.0	2816.0	2816.0	0.0	4852.6	4852.6	0.0	4852.6	0.0	0.0	0.0	0.0	0.0
Substream: NC																							
Mass Flow kg/hr																							
BIOMASS	61511.2	0.0	61511.2	0.0	35695.0	25816.3	35695.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass Frac																							
BIOMASS	1.0	0.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	61511.2	0.0	61511.2	0.0	35695.0	25816.3	35695.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

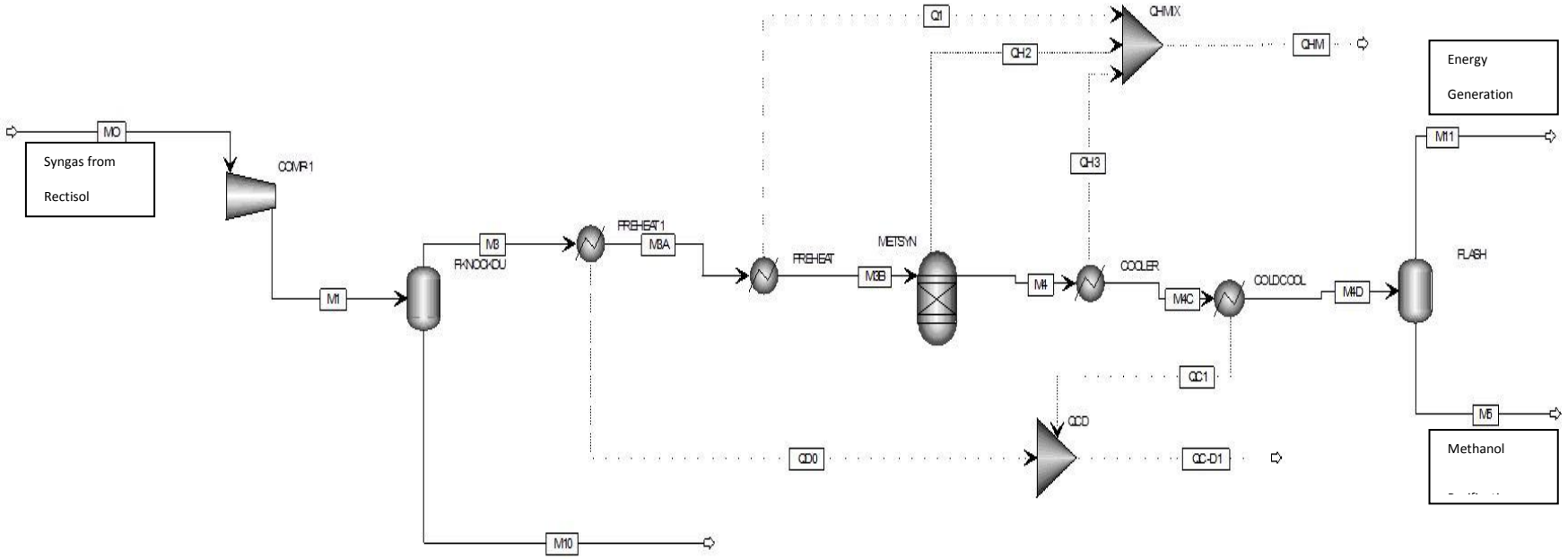
	G16	G16B	G17	G18	G19A	G19B	G19C	G20	G20A	G20B	G21	G21A	G22	G22A	G22B	G23	G23A	CLEANSYN	CO2VENT	CSNT2
Substream: MIXED																				
Mass Flow kg/hr																				
H2O	23916.7	23916.7	23916.7	6374.7	17542.0	5027.9	1033.2	6374.7	6374.7	6374.7	1346.7	1346.7	1346.7	1346.7	1346.7	313.5	313.5	0.0	172.2	313.5
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	26.4	26.4	26.4	26.4	0.0	0.0	0.0	26.4	26.4	26.4	26.4	26.4	26.4	26.4	26.4	26.4	26.4	25.8	0.6	26.4
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	20555.2	20555.2	20555.2	20554.7	0.4	0.6	0.5	20554.7	20554.7	20554.7	20554.2	20554.2	20554.2	20554.2	20554.2	20553.7	20553.7	1027.7	19525.9	20553.7
CO	22421.0	22421.0	22421.0	22421.0	0.0	0.0	0.0	22421.0	22421.0	22421.0	22421.0	22421.0	22421.0	22421.0	22421.0	22421.0	22421.0	21748.4	672.6	22421.0
H2	3531.7	3531.7	3531.7	3531.7	0.0	0.0	0.0	3531.7	3531.7	3531.7	3531.7	3531.7	3531.7	3531.7	3531.7	3531.7	3531.7	3499.9	31.8	3531.7
SO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	1.6	1.6	1.6	1.6	0.0	0.0	0.0	1.6	1.6	1.6	1.6	1.6	1.6	1.6	1.6	1.6	1.6	1.5	0.1	1.6
Total Flow kmol/hr	4348.1	4348.1	4348.1	3374.3	973.7	279.1	57.4	3374.3	3374.3	3374.3	3095.2	3095.2	3095.2	3095.2	3095.2	3037.9	3037.9	2537.0	493.0	3037.9
Total Flow kg/hr	70452.6	70452.6	70452.6	52910.2	17542.5	5028.5	1033.7	52910.2	52910.2	52910.2	47881.7	47881.7	47881.7	47881.7	47881.7	46848.0	46848.0	26303.2	20403.3	46848.0
Total Flow l/min	7023830.0	2037200.0	1450940.0	1495650.0	394.4	113.0	23.2	571341.0	416044.0	320363.0	326430.0	322555.0	128782.0	95407.7	78732.2	79842.9	79003.9	24965.6	703.7	50900.6
Temperature K	1181.2	342.9	318.2	324.2	324.2	323.2	321.0	519.3	378.2	318.2	323.2	319.6	507.8	378.2	318.2	321.0	319.0	234.4	234.4	399.0
Pressure atm	1.0	1.0	1.0	1.0	1.0	4.2	16.8	4.2	4.2	4.2	4.2	4.2	16.8	16.8	16.8	16.8	16.8	32.6	32.6	32.6
Vapor Frac	1.0	1.0	0.8	1.0	0.0	0.0	0.0	1.0	1.0	0.9	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.1	1.0
Liquid Frac	0.0	0.0	0.2	0.0	1.0	1.0	1.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.9	0.0
Substream: CISOLID																				
Mass Flow kg/hr																				
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASHO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Substream: NC																				
Mass Flow kg/hr																				
BIOMASS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass Frac																				
BIOMASS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

3.2 CONVENTIONAL METHANOL SYNTHESIS



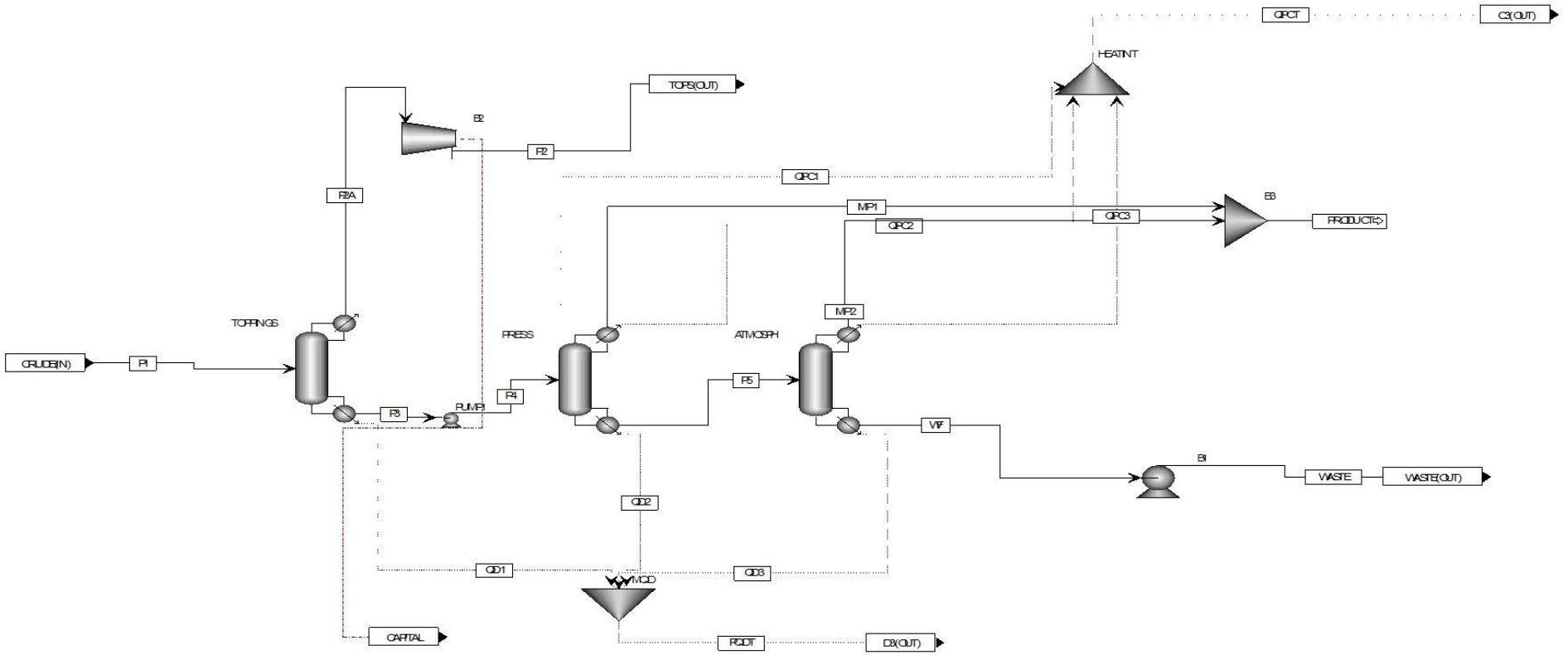
	M1	M2	M3	M4	M4C	M4D	M5	M6	M7	M8	M9	M10	M11	MO
Substream: MIXED														
Mass Flow kg/hr														
H2O	0.0	14.8	14.8	137.9	137.9	137.9	120.8	17.1	14.8	14.8	14.8	0.0	2.2	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	25.8	197.9	197.9	197.9	197.9	197.9	0.1	197.8	172.1	172.1	172.1	0.0	25.7	25.8
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	1027.7	5252.5	5252.5	4951.9	4952.0	4952.0	95.9	4856.1	4224.8	4224.8	4224.8	0.0	631.3	1027.7
CO	21748.4	64941.6	64941.6	49666.5	49666.1	49666.1	18.8	49647.4	43193.2	43193.2	43193.2	0.0	6454.2	21748.4
HCL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	3499.9	11918.3	11918.3	9678.3	9678.2	9678.2	1.9	9676.3	8418.4	8418.4	8418.4	0.0	1257.9	3499.9
ASHO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	1.5	11.4	11.4	11.4	11.4	11.4	0.0	11.4	9.9	9.9	9.9	0.0	1.5	1.5
C2H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
METOH	0.0	2677.3	2677.3	20369.9	20370.6	20370.6	17293.2	3077.4	2677.3	2677.3	2677.3	0.0	400.1	0.0
Total Flow kmol/hr	2537.0	8442.2	8442.2	7337.9	7337.8	7337.8	550.2	6787.6	5905.2	5905.2	5905.2	0.0	882.4	2537.0
Total Flow kg/hr	26303.2	85013.8	85013.8	85013.8	85014.0	85014.0	17530.6	67483.4	58710.5	58710.5	58710.5	0.0	8772.8	26303.2
Total Flow l/min	17042.0	68969.6	71187.3	114415.0	73098.9	57526.7	500.2	80865.5	69110.6	69723.5	51860.8	0.0	10326.9	24965.6
Temperature K	290.9	353.7	353.7	573.2	378.2	318.2	320.5	320.5	321.4	323.8	380.3		321.4	234.4
Pressure atm	59.2	59.2	59.2	51.3	51.3	51.3	37.5	37.5	37.5	37.5	59.2	59.2	37.5	32.6

3.3 ADVANCED METHANOL SYNTHESIS



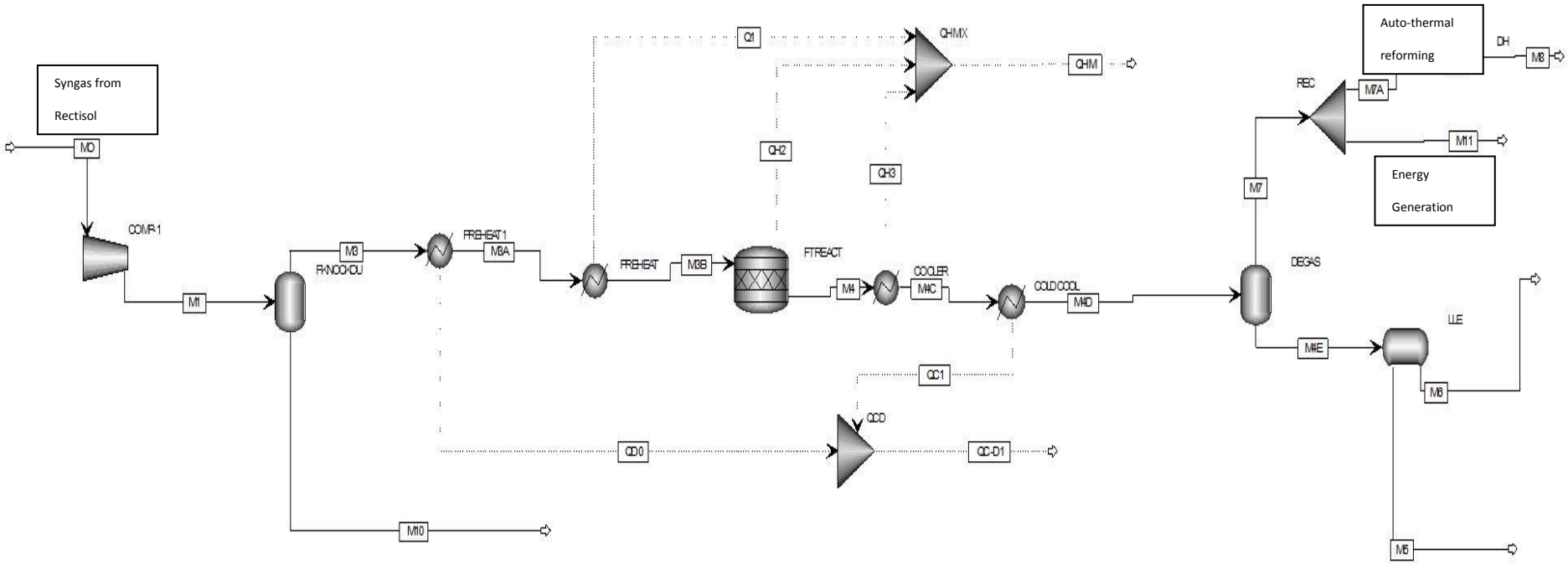
	MO	M1	M3	M3A	M3B	M4	M4C	M4D	M5	M10	M11
Substream: MIXED											
Mass Flow kg/hr											
H2O	0.0	0.0	0.0	0.0	0.0	18.6	18.6	18.6	18.2	0.0	0.4
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	25.8	25.8	25.8	25.8	25.8	25.8	25.8	25.8	0.1	0.0	25.6
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	1027.7	1027.7	1027.7	1027.7	1027.7	982.3	982.3	982.3	165.6	0.0	816.6
CO	21748.4	21748.4	21748.4	21748.4	21748.4	3971.0	3971.0	3971.0	22.0	0.0	3948.9
HCL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	3499.9	3499.9	3499.9	3499.9	3499.9	934.8	934.8	934.8	2.9	0.0	931.9
CH4	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	0.0	0.0	1.5
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
METOH	0.0	0.0	0.0	0.0	0.0	20369.3	20369.3	20369.3	19783.0	0.0	586.4
Total Flow kmol/hr	2537.0	2537.0	2537.0	2537.0	2537.0	1265.6	1265.6	1265.6	624.4	0.0	641.2
Total Flow kg/hr	26303.2	26303.2	26303.2	26303.2	26303.2	26303.2	26303.2	26303.2	19991.8	0.0	6311.4
Total Flow l/min	24965.6	12950.6	13620.9	15902.1	19417.6	9670.3	4225.9	3429.9	583.4	0.0	8004.7
Temperature K	234.4	338.9	338.5	416.2	508.2	523.2	378.2	318.2	336.4		336.4
Pressure atm	32.6	90.8	90.8	90.8	90.8	88.8	88.8	88.8	37.5	90.8	37.5
Vapor Frac	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.5	0.0		1.0
Liquid Frac	0.0	0.0	0.0	0.0	0.0	0.0	0.5	0.5	1.0		0.0

3.4 METHANOL PURIFICATION



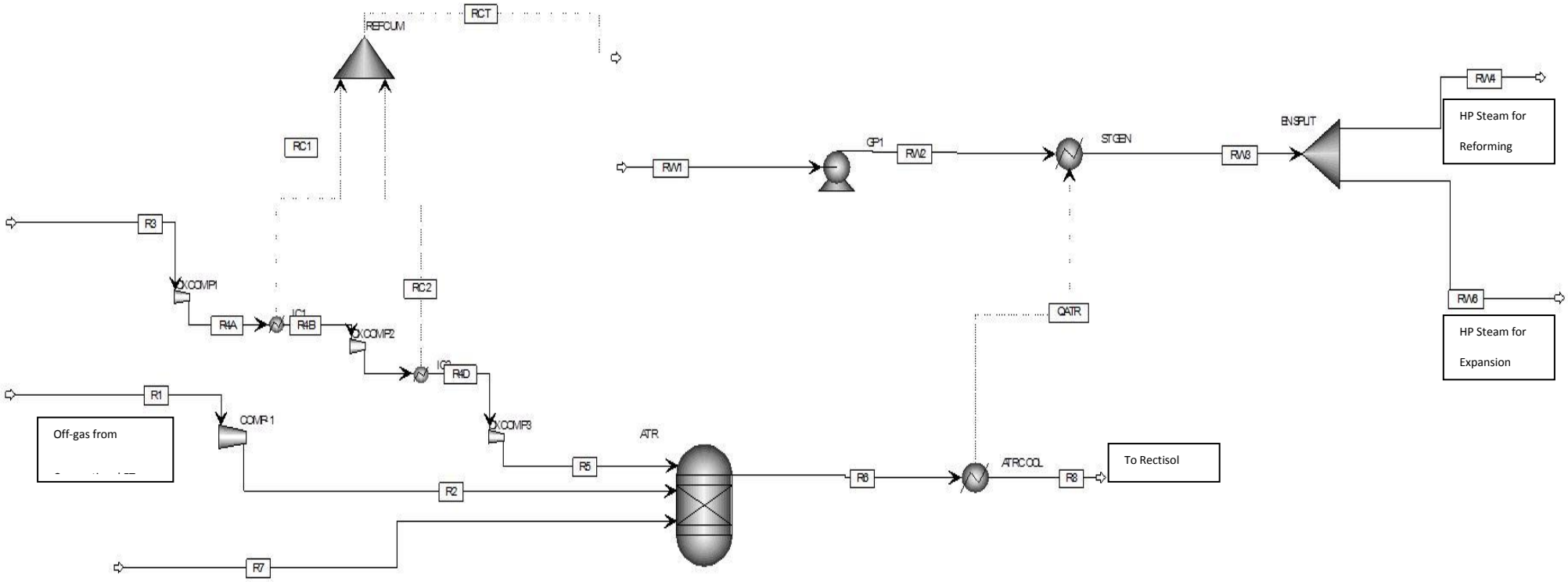
	MP1	MP2	P1	P2	P2A	P3	P4	P5	PRODUCT	WASTE	WF
Substream: MIXED											
Mass Flow kg/hr											
H2O	7.4	2.0	18.2	0.0	0.0	18.2	18.2	10.8	9.4	8.7	8.7
N2	0.0	0.0	0.1	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	165.6	165.6	165.6	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	22.0	22.0	22.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	2.9	2.9	2.9	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
METOH	9841.9	9743.5	19783.0	99.1	99.1	19683.9	19683.9	9841.9	19585.5	98.4	98.4
Total Flow kmol/hr	307.6	304.2	624.4	9.1	9.1	615.3	615.3	307.8	611.8	3.6	3.6
Total Flow kg/hr	9849.3	9745.5	19991.8	289.8	289.8	19702.0	19702.0	9852.7	19594.9	107.1	107.1
Total Flow l/min	23819.7	140496.0	583.4	328.5	2696.5	451.7	452.1	321.6	299280.0	2.4	2.4
Temperature K	392.7	337.7	336.4	613.3	321.3	350.7	351.2	393.5	357.7	350.5	347.8
Pressure atm	6.4	1.0	37.5	23.2	1.5	1.6	9.0	6.6	1.0	23.2	1.3
Vapor Frac	1.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0
Liquid Frac	0.0	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0	1.0	1.0

3.5 CONVENTIONAL FT SYNTHESIS



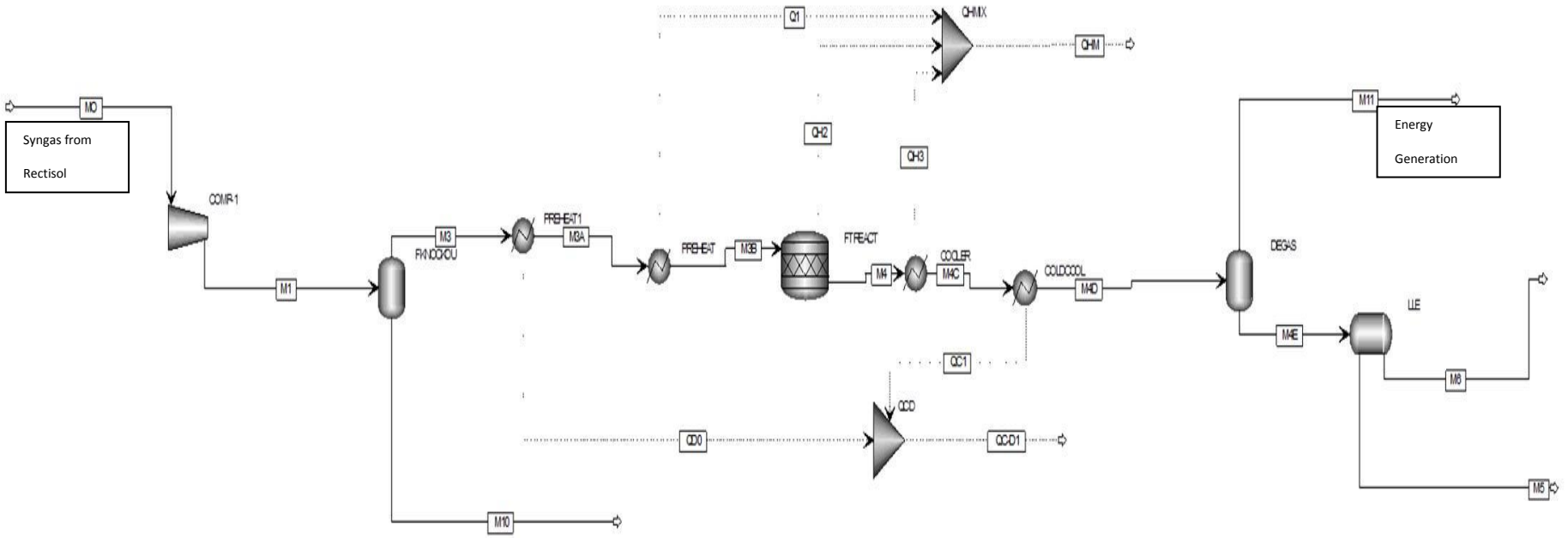
	MO	M1	M3	M3A	M3B	M4	M4C	M4D	M4E	M5	M6	M7	M7A	M8	M10	M11
Substream: MIXED																
Mass Flow kg/hr																
H2O	0.0	0.0	0.0	0.0	0.0	9567.0	9567.0	9567.0	9398.1	2.3	9395.7	168.9	118.3	118.3	0.0	50.7
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	142.5	142.5	142.5	142.5	142.5	142.5	142.5	142.5	1.2	0.3	0.9	141.3	98.9	98.9	0.0	42.4
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	1198.9	1198.9	1198.9	1198.9	1198.9	1198.9	1198.9	1198.9	133.3	56.9	76.4	1065.6	745.9	745.9	0.0	319.7
CO	37187.4	37187.4	37187.4	37187.4	37187.4	22312.4	22312.4	22312.4	241.9	52.8	189.2	22070.5	15449.3	15449.3	0.0	6621.1
HCL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	5714.9	5714.9	5714.9	5714.9	5714.9	3363.9	3363.9	3363.9	0.0	0.0	0.0	3363.9	2354.7	2354.7	0.0	1009.2
CH4	1099.7	1099.7	1099.7	1099.7	1099.7	2036.9	2036.9	2036.9	156.8	118.3	38.5	1880.1	1316.1	1316.1	0.0	564.0
C2H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
METOH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MGO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10	0.0	0.0	0.0	0.0	0.0	848.8	848.8	848.8	491.0	485.6	5.4	357.8	250.5	250.5	0.0	107.3
C9H20	0.0	0.0	0.0	0.0	0.0	1967.7	1967.7	1967.7	877.5	877.4	0.0	1090.2	763.1	763.1	0.0	327.1
C15H32	0.0	0.0	0.0	0.0	0.0	1955.3	1955.3	1955.3	1955.3	1955.3	0.0	0.0	0.0	0.0	0.0	0.0
C21H44	0.0	0.0	0.0	0.0	0.0	1950.0	1950.0	1950.0	1950.0	1950.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	4263.4	4263.4	4263.4	4263.4	4263.4	3201.3	3201.3	3201.3	574.2	41.7	532.6	2627.1	1839.0	1839.0	0.0	788.1
Total Flow kg/hr	45343.4	45343.4	45343.4	45343.4	45343.4	45343.4	45343.4	45343.4	15205.0	5499.0	9706.0	30138.4	21096.9	21096.9	0.0	9041.5
Total Flow l/min	43266.3	36369.8	37437.4	58537.7	71478.9	56816.5	35744.1	29246.2	314.3	143.5	168.0	49632.2	34938.7	38535.2	0.0	14973.7
Temperature K	234.4	258.6	260.9	416.2	508.2	513.2	378.2	318.2	315.1	316.0	316.0	315.1	320.8	352.3		320.8
Pressure atm	31.6	41.5	41.5	41.5	41.5	39.5	39.5	39.5	23.0	23.0	23.0	23.0	23.0	23.0	41.5	23.0
Vapor Frac	1.0	1.0	1.0	1.0	1.0	1.0	0.8	0.8	0.0	0.0	0.0	1.0	1.0	1.0		1.0
Liquid Frac	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.2	1.0	1.0	1.0	0.0	0.0	0.0		0.0

3.6 RECYCLE GAS REFORMING



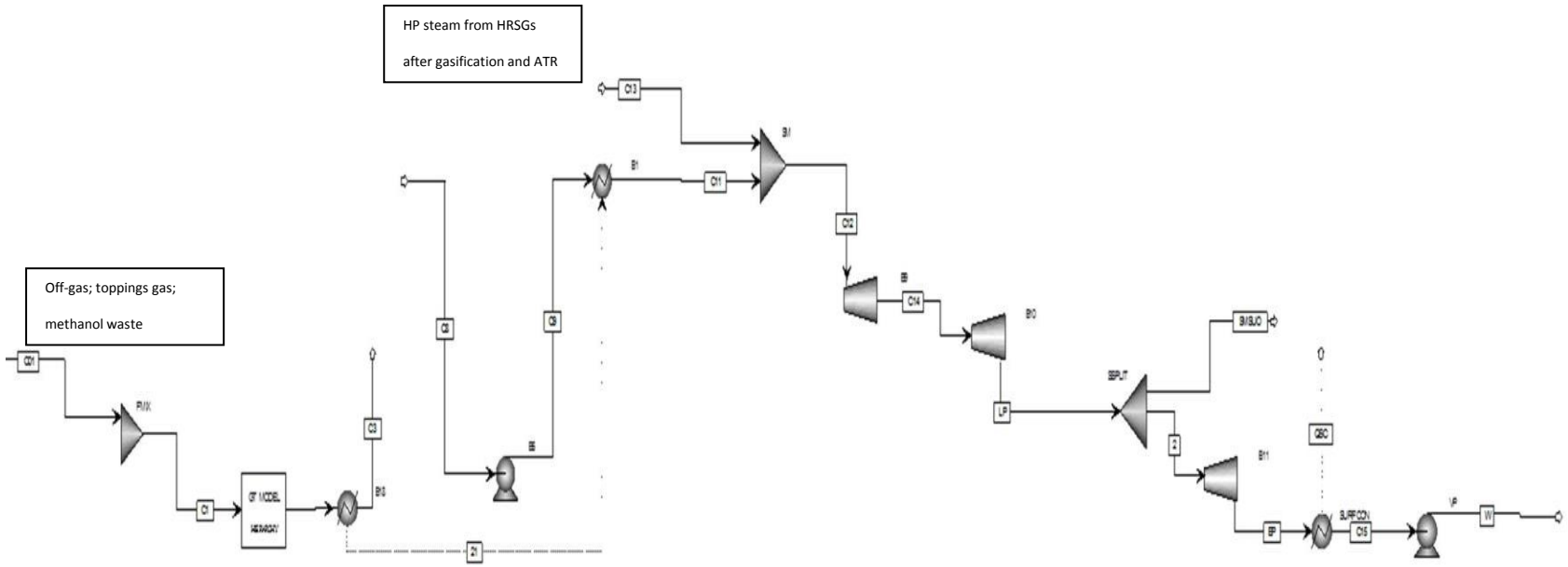
	R 1	R 2	R 3	R4A	R4B	R4C	R4D	R 5	R 6	R 7	R 8	RW1	RW2	RW3	RW4	RW6
Substream: MIXED																
Mass Flow kg/hr																
H2O	118.3	118.3	0.0	0.0	0.0	0.0	0.0	0.0	4555.5	1662.7	4555.5	17422.3	17422.3	17422.3	1661.3	15761.0
O2	0.0	0.0	4680.0	4680.0	4680.0	4680.0	4680.0	4680.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	98.9	98.9	20.7	20.7	20.7	20.7	20.7	20.7	119.6	0.0	119.6	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	745.9	745.9	0.0	0.0	0.0	0.0	0.0	0.0	3426.7	0.0	3426.7	0.0	0.0	0.0	0.0	0.0
CO	15449.3	15449.3	0.0	0.0	0.0	0.0	0.0	0.0	15916.5	0.0	15916.5	0.0	0.0	0.0	0.0	0.0
HCL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	2354.7	2354.7	0.0	0.0	0.0	0.0	0.0	0.0	2235.1	0.0	2235.1	0.0	0.0	0.0	0.0	0.0
CH4	1316.1	1316.1	0.0	0.0	0.0	0.0	0.0	0.0	1206.9	0.0	1206.9	0.0	0.0	0.0	0.0	0.0
C2H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10	250.5	250.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C9H20	763.1	763.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C15H32	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C21H44	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	1839.0	1839.0	147.0	147.0	147.0	147.0	147.0	147.0	2087.2	92.3	2087.2	967.1	967.1	967.1	92.2	874.9
Total Flow kg/hr	21096.9	21096.9	4700.7	4700.7	4700.7	4700.7	4700.7	4700.7	27460.3	1662.7	27460.3	17422.3	17422.3	17422.3	1661.3	15761.0
Total Flow l/min	38535.2	30612.1	18730.4	15557.4	15248.3	6088.4	4050.3	2512.3	116046.0	802.1	37544.5	293.6	295.4	9129.8	870.6	8259.2
Temperature K	352.3	396.4	298.2	324.6	318.2	478.2	318.2	394.7	1276.9	845.2	415.8	303.2	309.5	845.5	845.5	845.5
Pressure atm	23.0	32.6	3.2	4.2	4.2	15.8	15.8	31.6	31.6	122.5	31.6	1.0	122.5	122.5	122.5	122.5
Vapor Frac	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0
Liquid Frac	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0

3.7 ADVANCED FT SYNTHESIS



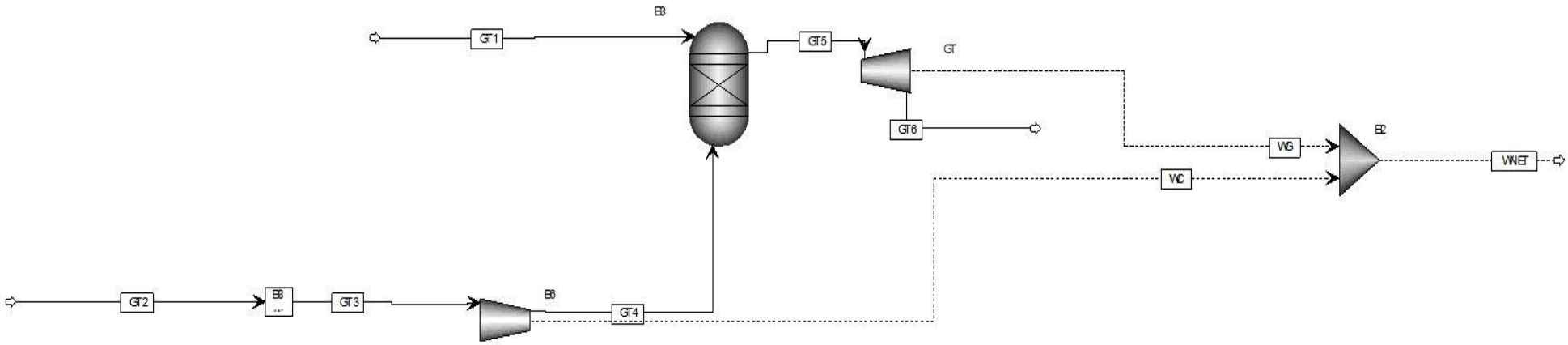
	MO	M1	M3	M3A	M3B	M4	M4C	M4D	M4E	M5	M6	M10	M11
Substream: MIXED													
Mass Flow kg/hr													
H2O	0.0	0.0	0.0	0.0	0.0	11190.2	11190.2	11190.2	11145.5	5.2	11140.4	0.0	44.7
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	25.8	25.8	25.8	25.8	25.8	25.8	25.8	25.8	1.2	0.3	0.9	0.0	24.6
NO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	1027.7	1027.7	1027.7	1027.7	1027.7	1027.7	1027.7	1027.7	433.2	208.4	224.9	0.0	594.4
CO	21748.4	21748.4	21748.4	21748.4	21748.4	4349.7	4349.7	4349.7	252.2	65.2	186.9	0.0	4097.5
H2	3499.9	3499.9	3499.9	3499.9	3499.9	750.0	750.0	750.0	0.0	0.0	0.0	0.0	750.0
CH4	1.5	1.5	1.5	1.5	1.5	1097.6	1097.6	1097.6	358.2	282.7	75.5	0.0	739.4
C4H10	0.0	0.0	0.0	0.0	0.0	992.8	992.8	992.8	876.0	868.0	8.0	0.0	116.9
C9H20	0.0	0.0	0.0	0.0	0.0	2301.5	2301.5	2301.5	1982.3	1982.3	0.1	0.0	319.2
C15H32	0.0	0.0	0.0	0.0	0.0	2287.0	2287.0	2287.0	2287.0	2287.0	0.0	0.0	0.0
C21H44	0.0	0.0	0.0	0.0	0.0	2280.8	2280.8	2280.8	2280.8	2280.8	0.0	0.0	0.0
Total Flow kmol/hr	2537.0	2537.0	2537.0	2537.0	2537.0	1294.7	1294.7	1294.7	708.9	73.8	635.0	0.0	585.8
Total Flow kg/hr	26303.2	26303.2	26303.2	26303.2	26303.2	26303.2	26303.2	26303.2	19616.5	7979.9	11636.6	0.0	6686.8
Total Flow l/min	24965.6	21408.4	22038.1	34833.1	42533.8	22366.9	8686.4	7037.8	415.4	215.6	202.4	0.0	11184.3
Temperature K	234.4	255.8	257.9	416.2	508.2	513.2	378.2	318.2	318.8	320.1	320.1		318.8
Pressure atm	32.6	41.5	41.5	41.5	41.5	39.5	39.5	39.5	23.0	23.0	23.0	41.5	23.0
Vapor Frac	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.5	0.0	0.0	0.0		1.0
Liquid Frac	0.0	0.0	0.0	0.0	0.0	0.0	0.5	0.5	1.0	1.0	1.0		0.0

3.8 ENERGY GENERATION



	C01	C1	C3	C8	C9	C11	C12	C13	C14	C15
Mass Flow kg/hr										
H2O	44.7	44.7	9037.5	31064.6	31064.6	31064.6	90130.0	59065.4	90130.0	30864.1
O2	0.0	0.0	25418.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	24.6	24.6	124586.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO2	0.0	0.0	6.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NO	0.0	0.0	328.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	594.4	594.4	12716.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	4097.5	4097.5	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HCL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	750.0	750.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	739.4	739.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10	116.9	116.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C9H20	319.2	319.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C15H32	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C21H44	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	585.8	585.8	6043.4	1724.3	1724.3	1724.3	5003.0	3278.6	5003.0	1713.2
Total Flow kg/hr	6686.8	6686.8	172093.0	31064.6	31064.6	31064.6	90130.0	59065.4	90130.0	30864.1
Total Flow l/min	11184.3	11287.9	2816670.0	523.4	524.6	14954.0	45913.6	30840.9	176943.0	536.1
Temperature K	318.8	325.7	363.2	303.2	305.4	843.8	821.9	842.4	630.8	333.2
Pressure atm	23.0	23.0	1.1	1.0	122.5	122.5	122.5	122.5	23.3	0.2
Vapor Frac	1.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0	1.0	0.0
Liquid Frac	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	1.0

3.9 GT MODEL



	GT1	GT2	GT3	GT4	GT5	GT6
Substream: MIXED						
Mass Flow kg/hr						
H2O	44.7	0.0	0.0	0.0	9037.5	9037.5
O2	0.0	18264.0	38374.3	38374.3	25418.9	25418.9
N2	24.6	59358.0	124716.0	124716.0	124586.0	124586.0
NO2	0.0	0.0	0.0	0.0	6.2	6.2
NO	0.0	0.0	0.0	0.0	328.5	328.5
CO2	594.4	1102.1	2315.7	2315.7	12716.1	12716.1
CO	4097.5	0.0	0.0	0.0	0.1	0.1
HCL	0.0	0.0	0.0	0.0	0.0	0.0
H2	750.0	0.0	0.0	0.0	0.0	0.0
CL2	0.0	0.0	0.0	0.0	0.0	0.0
SO	0.0	0.0	0.0	0.0	0.0	0.0
SO2	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0
SO3	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0
ASHO	0.0	0.0	0.0	0.0	0.0	0.0
CH4	739.4	0.0	0.0	0.0	0.0	0.0
C2H4	0.0	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0
METOH	0.0	0.0	0.0	0.0	0.0	0.0
MGO	0.0	0.0	0.0	0.0	0.0	0.0
C4H10	116.9	0.0	0.0	0.0	0.0	0.0
C9H20	319.2	0.0	0.0	0.0	0.0	0.0
C15H32	0.0	0.0	0.0	0.0	0.0	0.0
C21H44	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kmol/hr	585.8	2714.7	5703.9	5703.9	6043.4	6043.4
Total Flow kg/hr	6686.8	78724.1	165406.0	165406.0	172093.0	172093.0
Total Flow l/min	11287.9	1106930.0	2325750.0	272562.0	702905.0	7127820.0
Temperature K	325.7	298.2	298.2	804.6	1631.3	918.5
Pressure atm	23.0	1.0	1.0	23.2	19.2	1.1
Vapor Frac	1.0	1.0	1.0	1.0	1.0	1.0
Liquid Frac	0.0	0.0	0.0	0.0	0.0	0.0

4. Appendix D4

Table D 16: : Configuration of flow sheets for Chapter 7 (30DS-- SSL substrate concentrated to a dissolved solid concentration of 30%; ME- Multi-effect distillation; CON – conventional distillation; MTOH-methanol synthesis; FT – Fischer-Tropsch synthesis;)

	Overall Scenarios	Subsections/Component flow-sheets									
		Ethanol Production; 30% Solids substrate; Conventional Distillation; Energy Recovery [A]	Ethanol Production; 30% Solids substrate; Multi-effect Distillation; Energy Recovery [A]	Biomass Boilers [A]	Biomass Integrated Gasification and Combined Cycles [B]	Gasification and Syngas Conditioning [C]	Advanced Methanol Synthesis loop [C]	Advanced Fischer-Tropsch synthesis loop [C]	Methanol Purification [C]	Energy Generation Circuit [C]	Gas Turbine Model [C]
Flow Sheets	30DS-CON BTE	x		x							
	30DS-ME-BTE		x	x							
	30DS-ME-BIGCC		x		x						
	30DS-CON-MTOH	x				X	X		X	X	X
	30DS-CON-FT	x				X		X		X	X

A. See Appendix D2
B. See Appendix D1
C. See Appendix D3

The flow-sheets of the overall scenarios in this chapter is a culmination of subsection flow-sheets already shown in Appendices D1-D3 and therefore, the component flow-sheets will not be reproduced here. The component flow-sheets referred from Appendix D2 (marked as “A” in Table D-4) were taken as is, whereas the component flow-sheets referred from Appendix D1 and Appendix D3 are adjusted for a different feedstock